

SUPPLEMENTARY MATERIAL

Polyketide Derivatives, guhypoxylonols A-D from a mangrove endophytic fungus *Aspergillus* sp. GXNU-Y45 that inhibit nitric oxide production

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Abstract: Four undescribed compounds, guhypoxylonols A (**1**), B (**2**), C (**3**), and D (**4**), were isolated from the mangrove endophytic fungus *Aspergillus* sp. GXNU-Y45, together with seven previously reported metabolites. The structures of **1-4** were elucidated based on analysis of HRESIMS data, NMR spectroscopic data. The absolute configurations of the stereogenic carbons in **1-3** were established through a combination of spectroscopic data and electronic circular dichroism (ECD). Compounds **1-11** were evaluated for their anti-inflammatory activity. Compounds **1**, **3**, **4**, and **6** showed an inhibitory activity against the production of nitric oxide (NO), with the IC₅₀ values of 14.42 ± 0.11, 18.03 ± 0.14, 16.66 ± 0.21, and 21.05 ± 0.13 μM, respectively.

Keywords: *Aspergillus* sp.; mangrove endophytic fungus; guhypoxylonols A-D; anti-inflammatory

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Table S2. Energy minimized coordinates of **1-2** model at the basis set def-SV(P) for all atoms(Å). **Figure S42.** ECD calculation of **2**

Table S3. Energy minimized coordinates of **2-1** model at the basis set def-SV(P) for all atoms(Å).

Table S4. Energy minimized coordinates of **2-2** model at the basis set def-SV(P) for all atoms(Å).

Table S5. Energy minimized coordinates of **2-3** model at the basis set def-SV(P) for all atoms(Å).

Table S6. Energy minimized coordinates of **2-4** model at the basis set def-SV(P) for all atoms(Å).

Table S7. Energy minimized coordinates of **2-5** model at the basis set def-SV(P) for all atoms(Å). **Table 8.** Energy minimized coordinates of **2-6** model at the basis set def-SV(P) for all atoms(Å).

Figure S43. ECD calculation of **3**

Table S9. Energy minimized coordinates of **3-1** model at the basis set def-SV(P) for all atoms(Å).

Table S10. Energy minimized coordinates of **3-2** model at the basis set def-SV(P) for all atoms(Å).

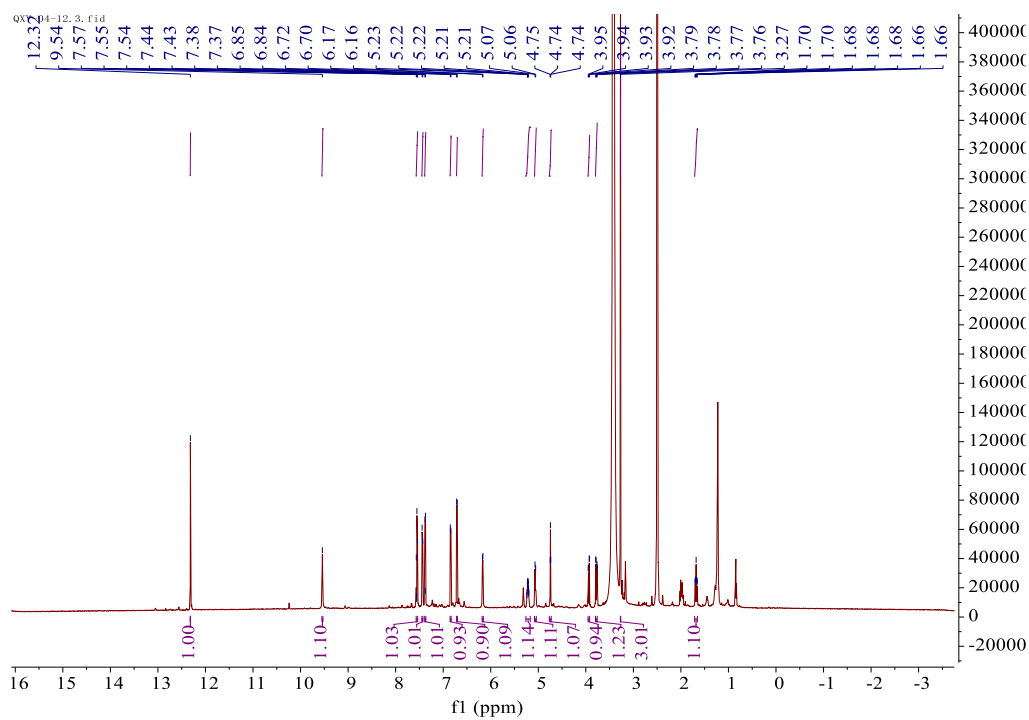


Figure S1. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of compound 1

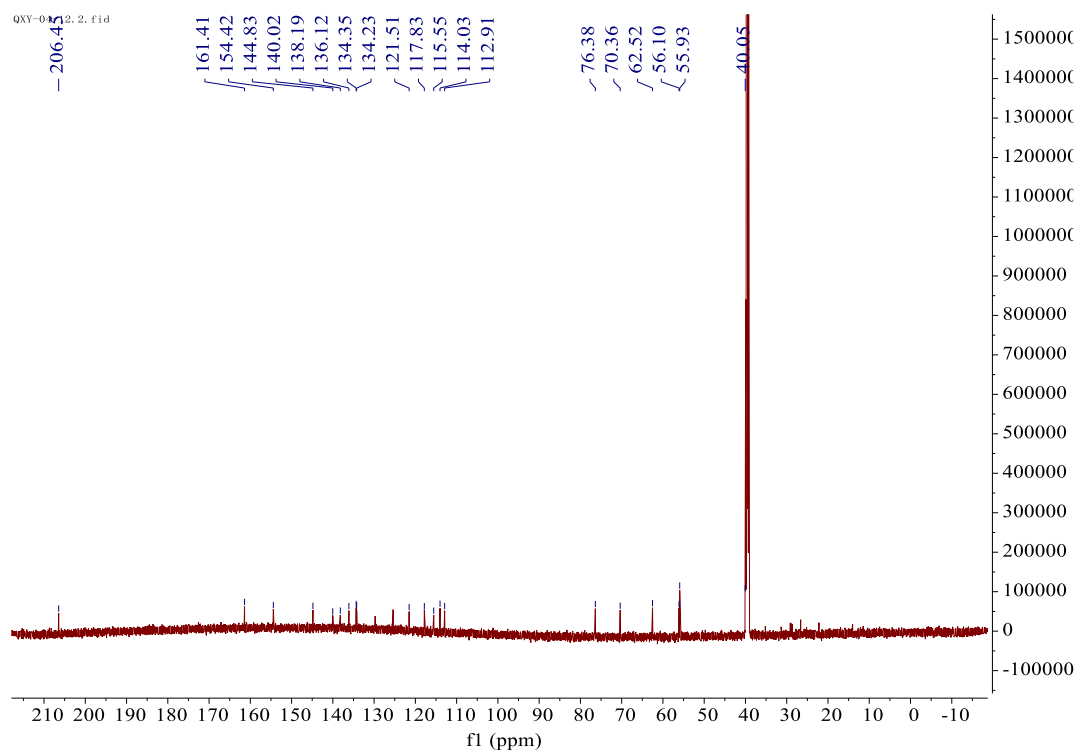


Figure S2. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of compound 1

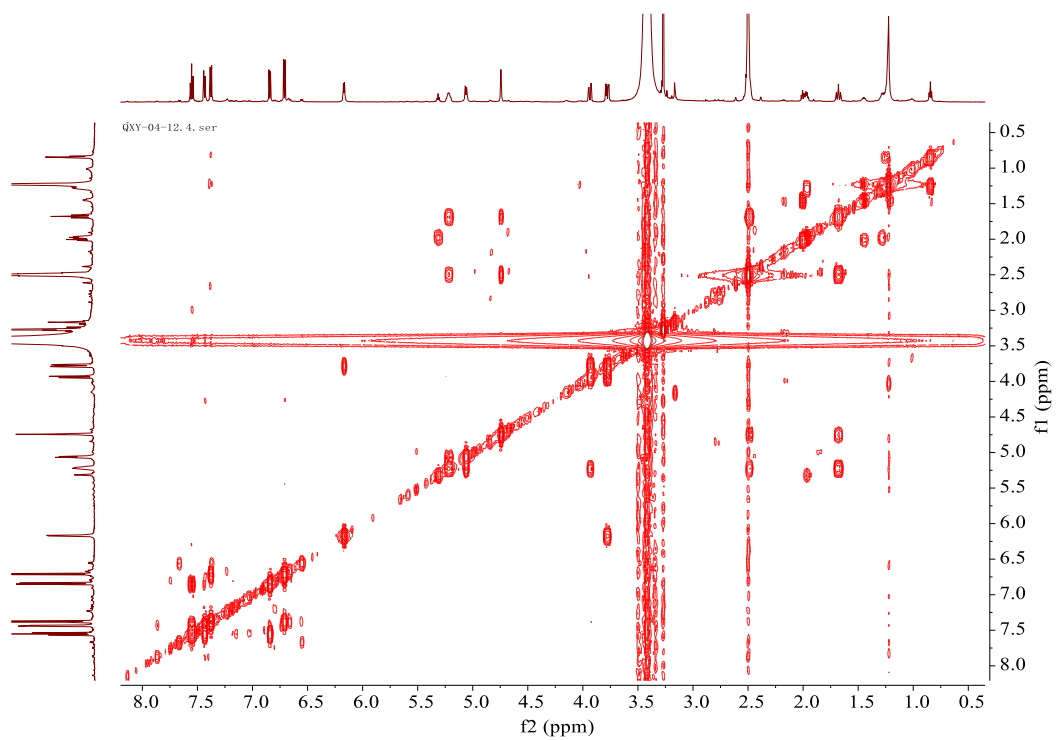


Figure S3. ^1H - ^1H COSY ($\text{DMSO}-d_6$) spectrum of compound **1**

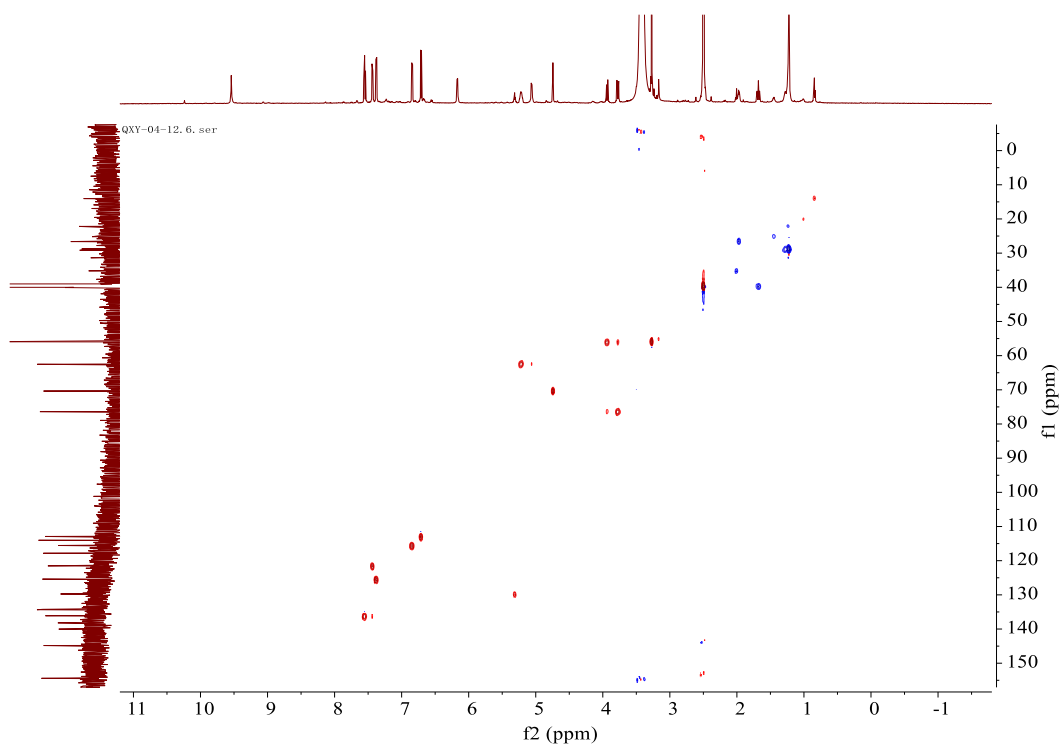


Figure S4. HMQC ($\text{DMSO}-d_6$) spectrum of compound **1**

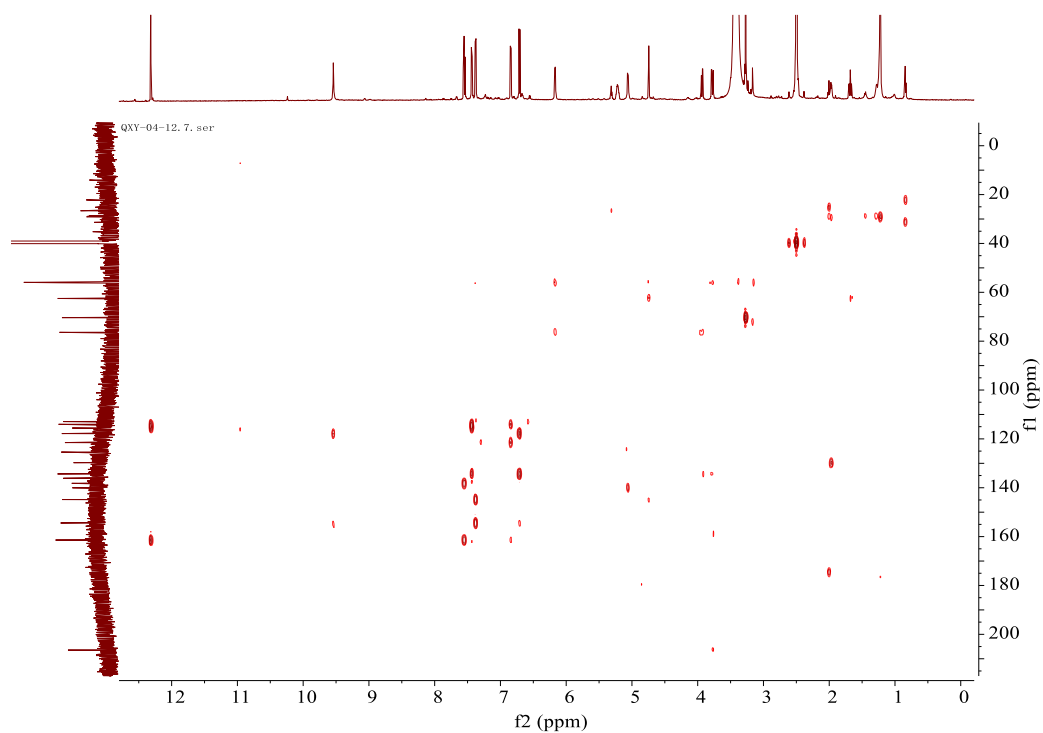


Figure S5. HMBC (DMSO- d_6) spectrum of compound **1**

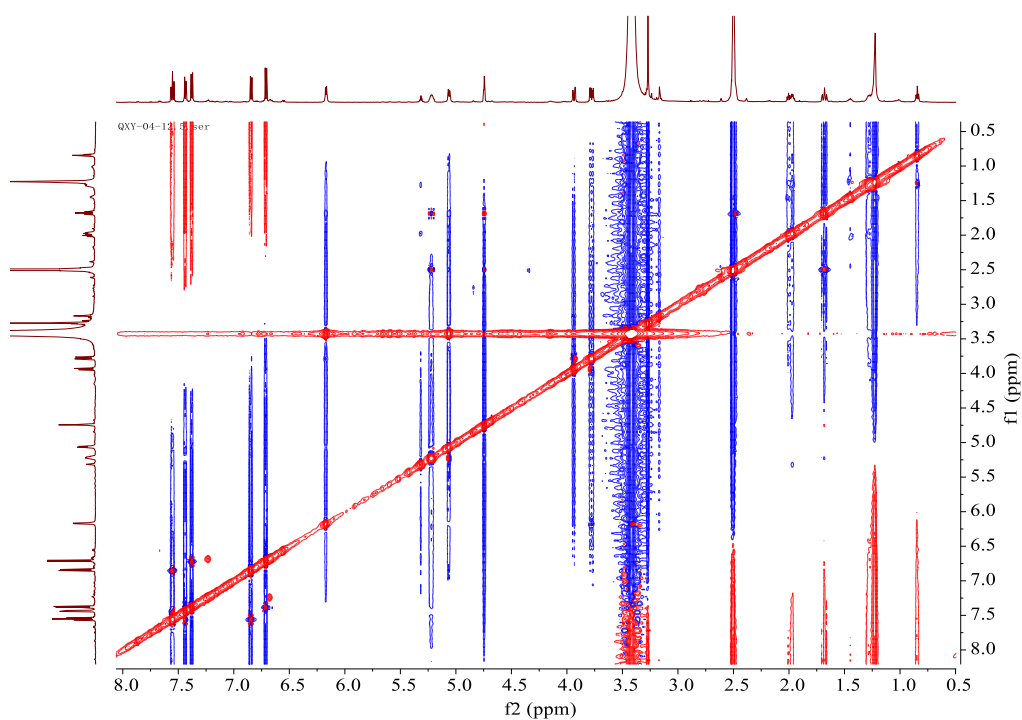


Figure S6. NOESY (DMSO- d_6) spectrum of compound **1**

Sample Name	04-12	Position	PLM	Instrument Name	Instrument 1
User Name		Inj Vol	0.3	Inj Position	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	04-12.d
ACQ Method	10-100% jiajun Zheng.m	Comment		Acquired Time	5/17/2021 5:11:58 PM

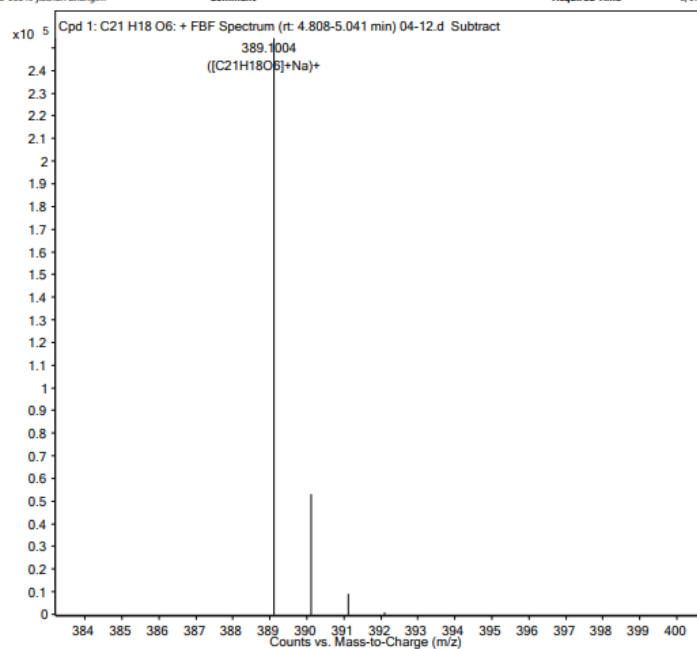


Figure S7. HR-ESI-MS spectrum of compound **1**

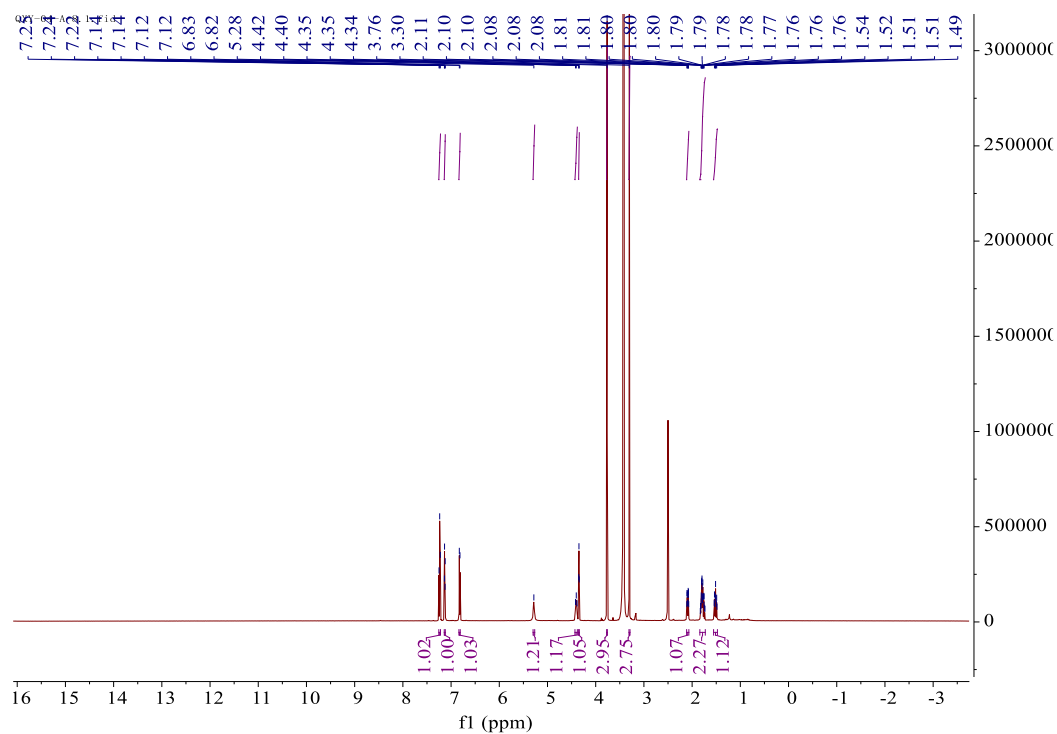


Figure S8. ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of compound **2**

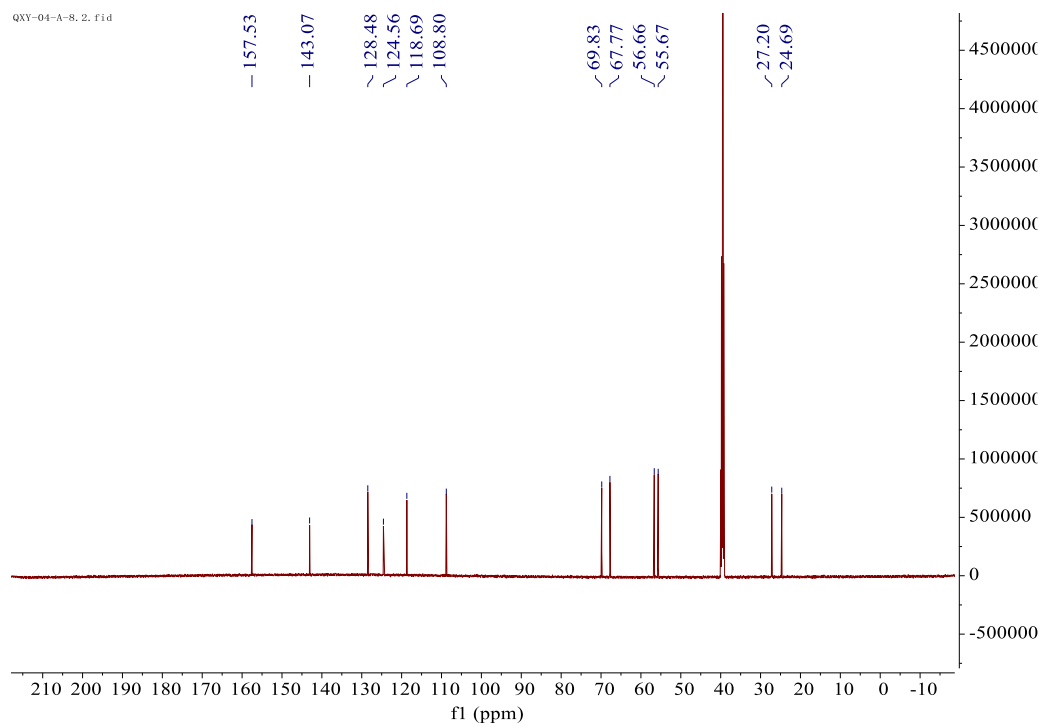


Figure S9. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of compound **2**

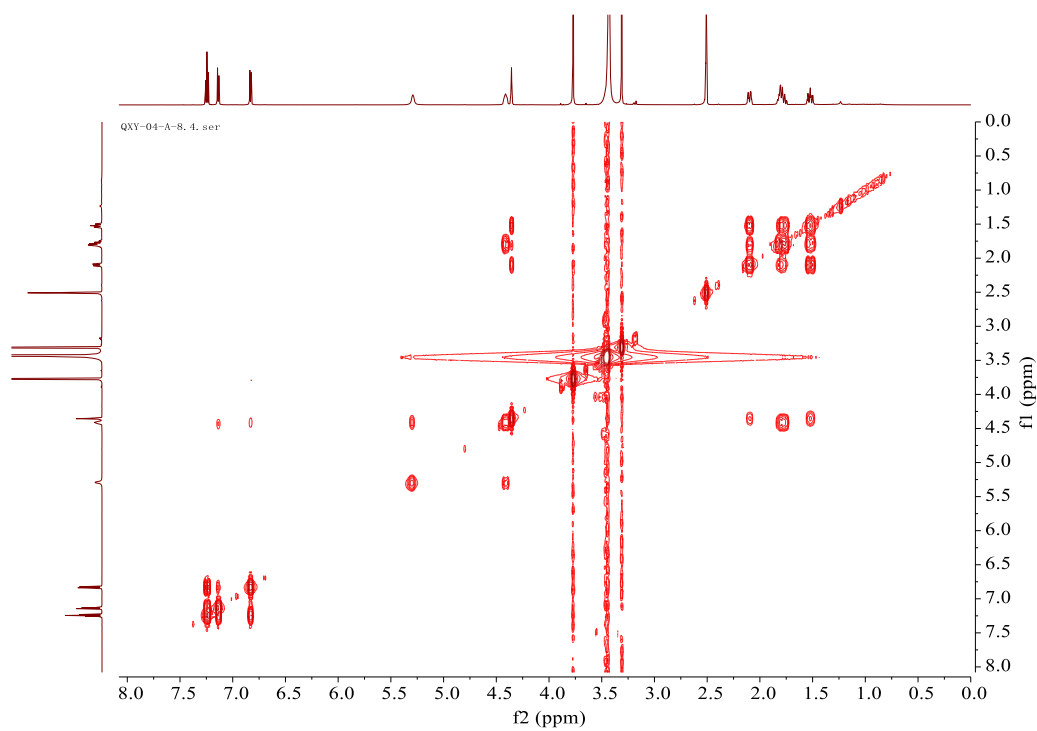


Figure S10. ^1H - ^1H COSY ($\text{DMSO}-d_6$) spectrum of compound **2**

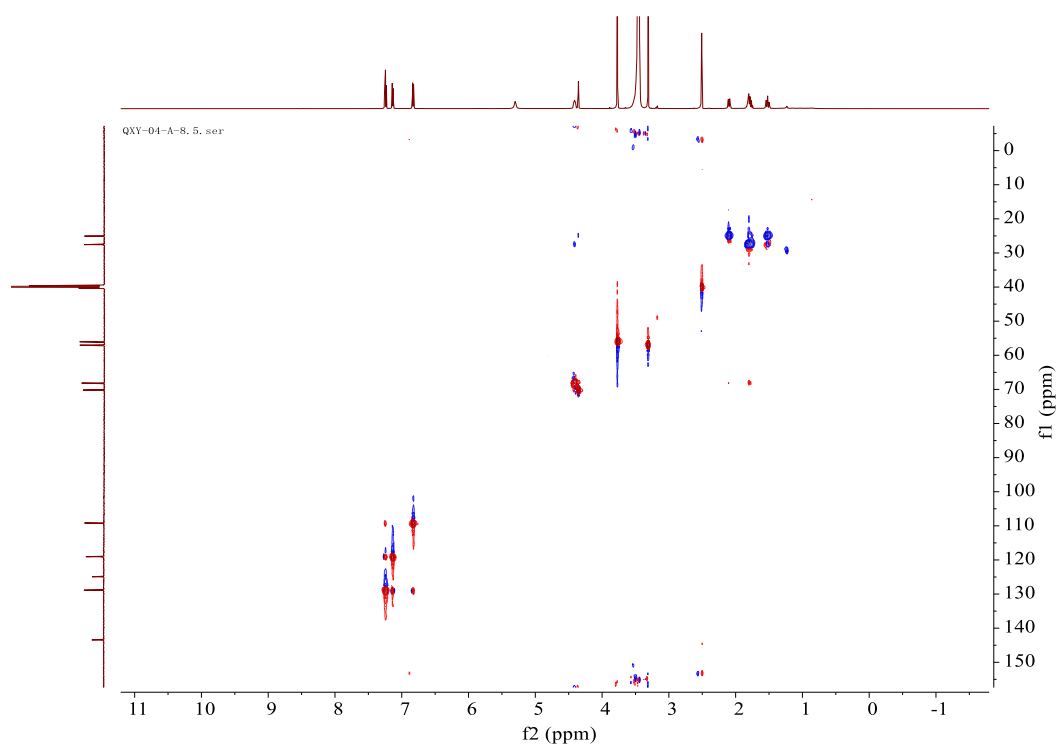


Figure S11. HMBC (DMSO- d_6) spectrum of compound **2**

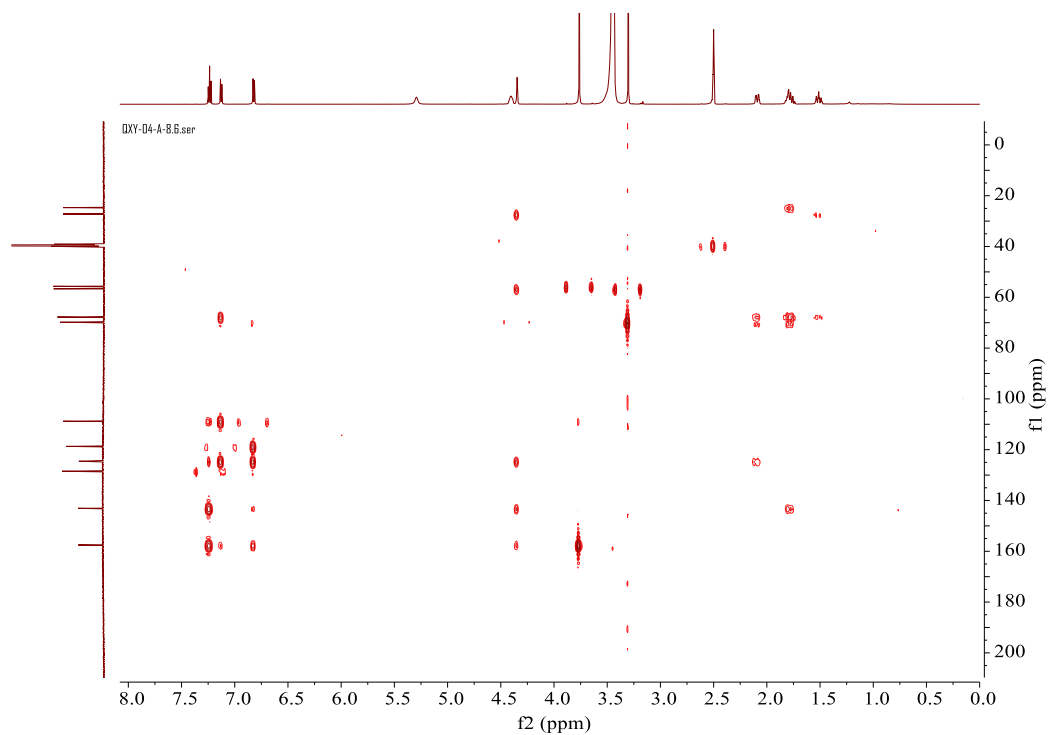


Figure S12. HMBC (DMSO- d_6) spectrum of compound **2**

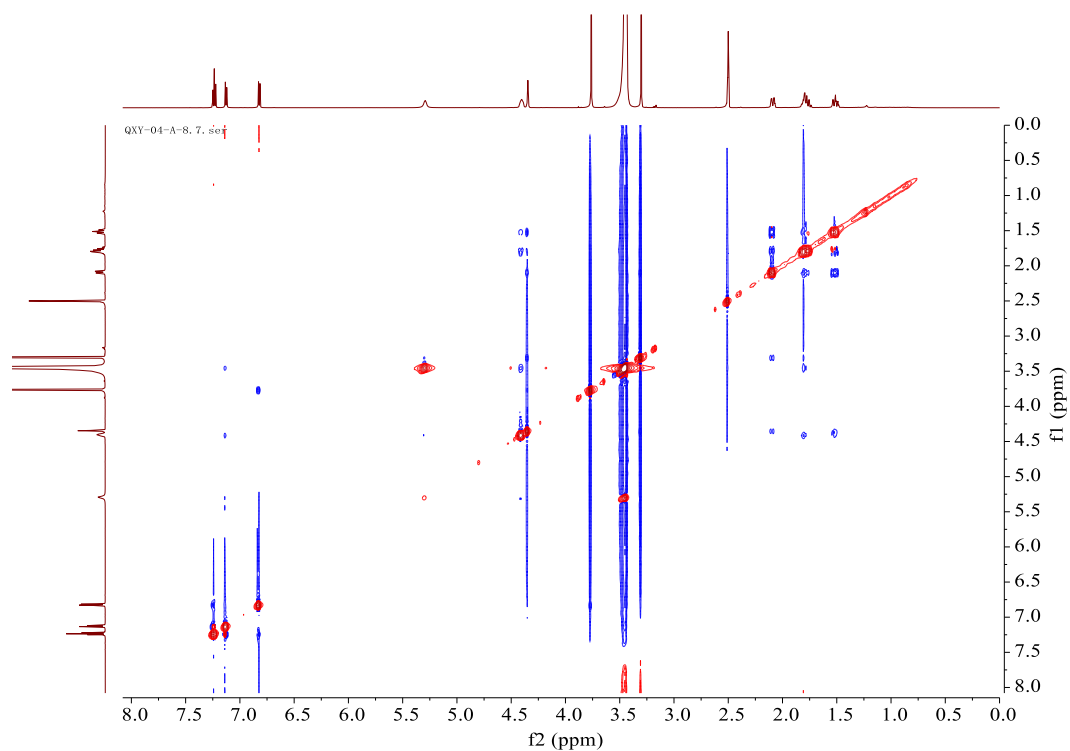


Figure S13. NOESY (DMSO- d_6) spectrum of compound **2**

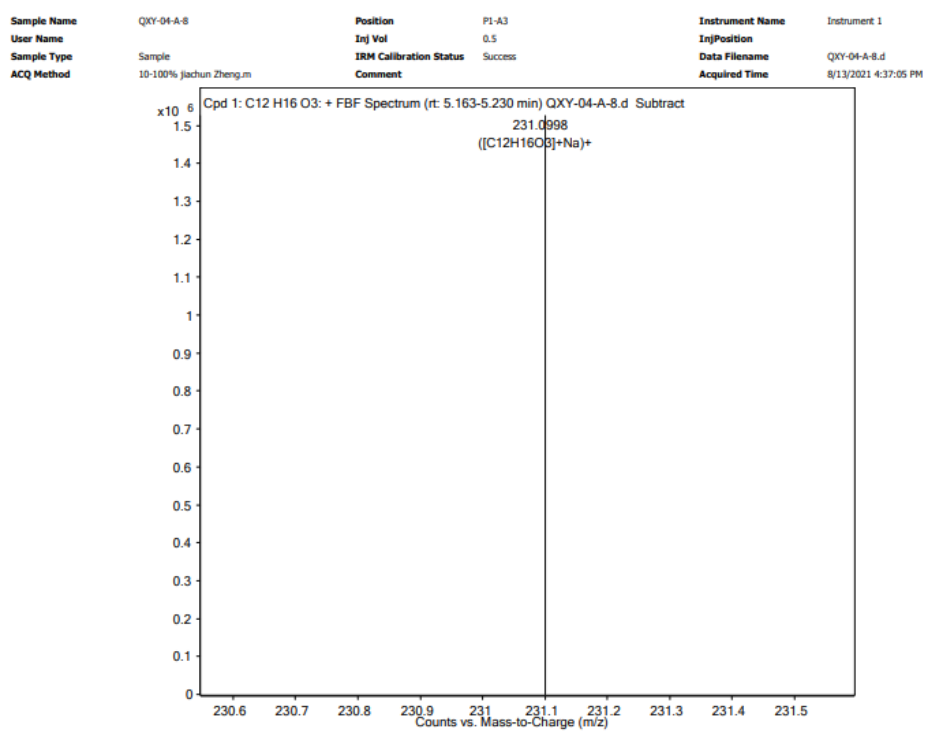


Figure S14. HR-ESI-MS spectrum of compound **2**

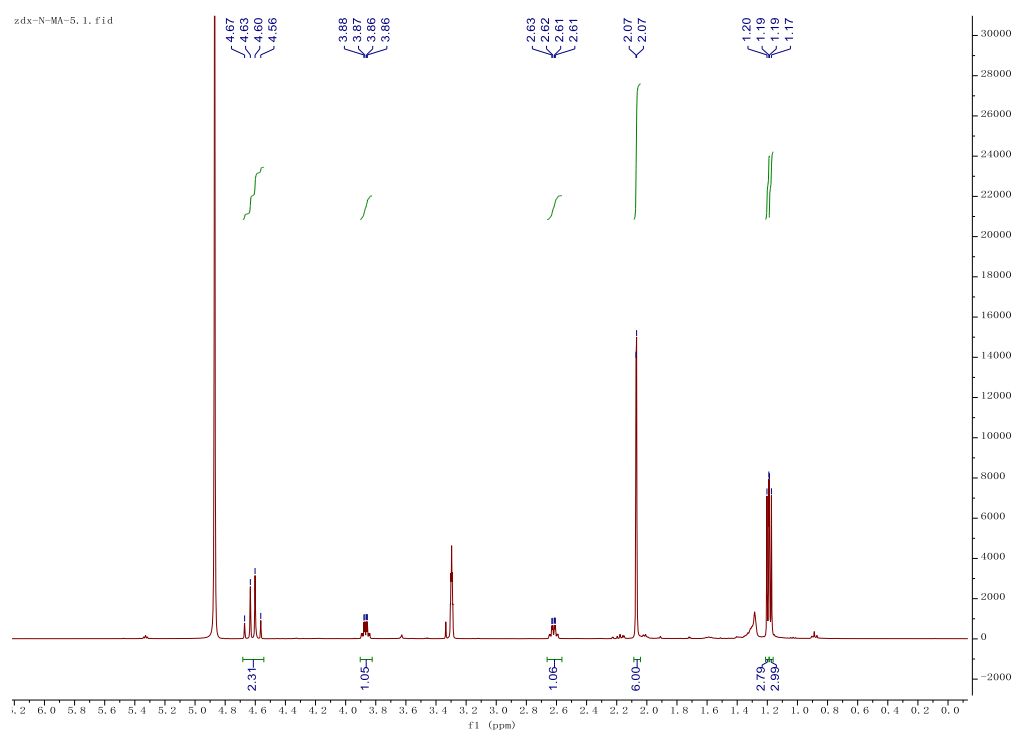


Figure S15. ^1H NMR (400 MHz, methanol- d_4) spectrum of compound **3**

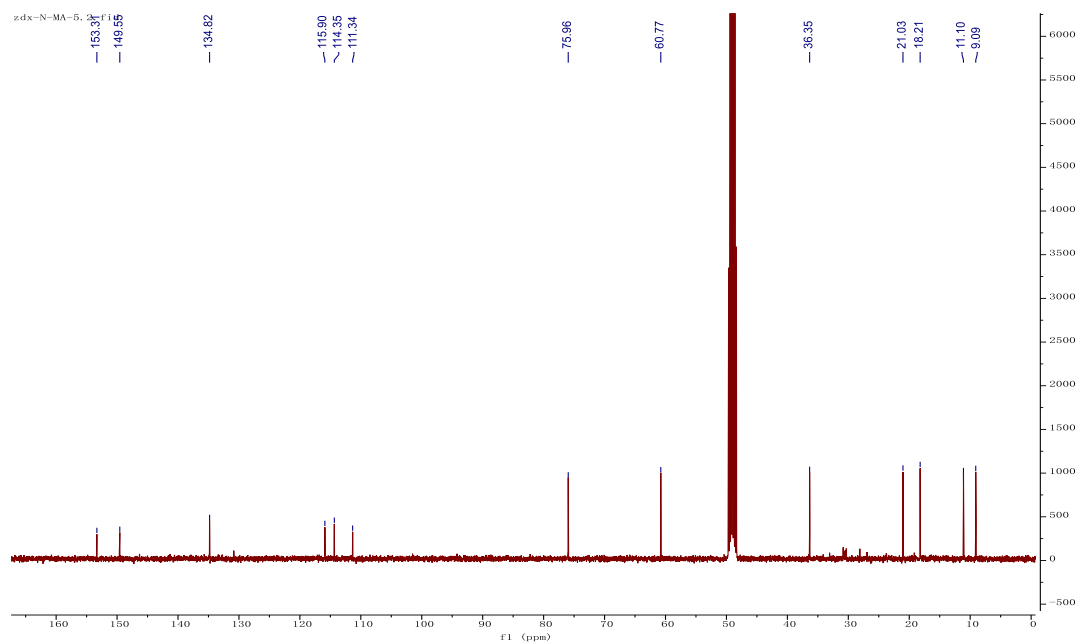


Figure S16. ^{13}C NMR (100 MHz, methanol- d_4) spectrum of compound **3**

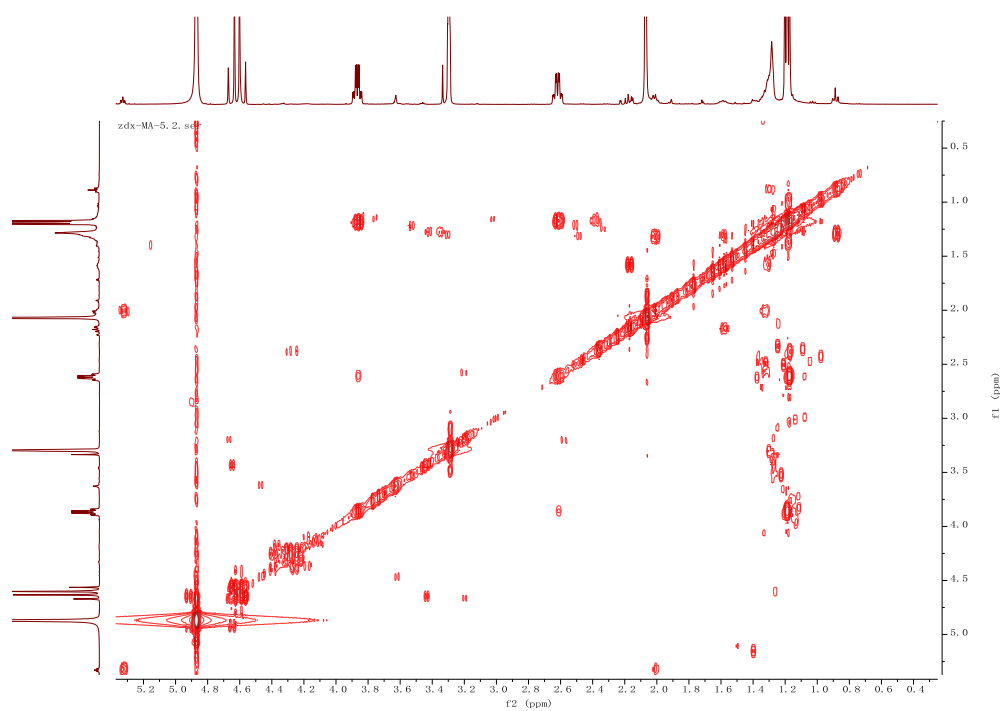


Figure S17. ^1H - ^1H COSY (methanol- d_4) spectrum of compound **3**

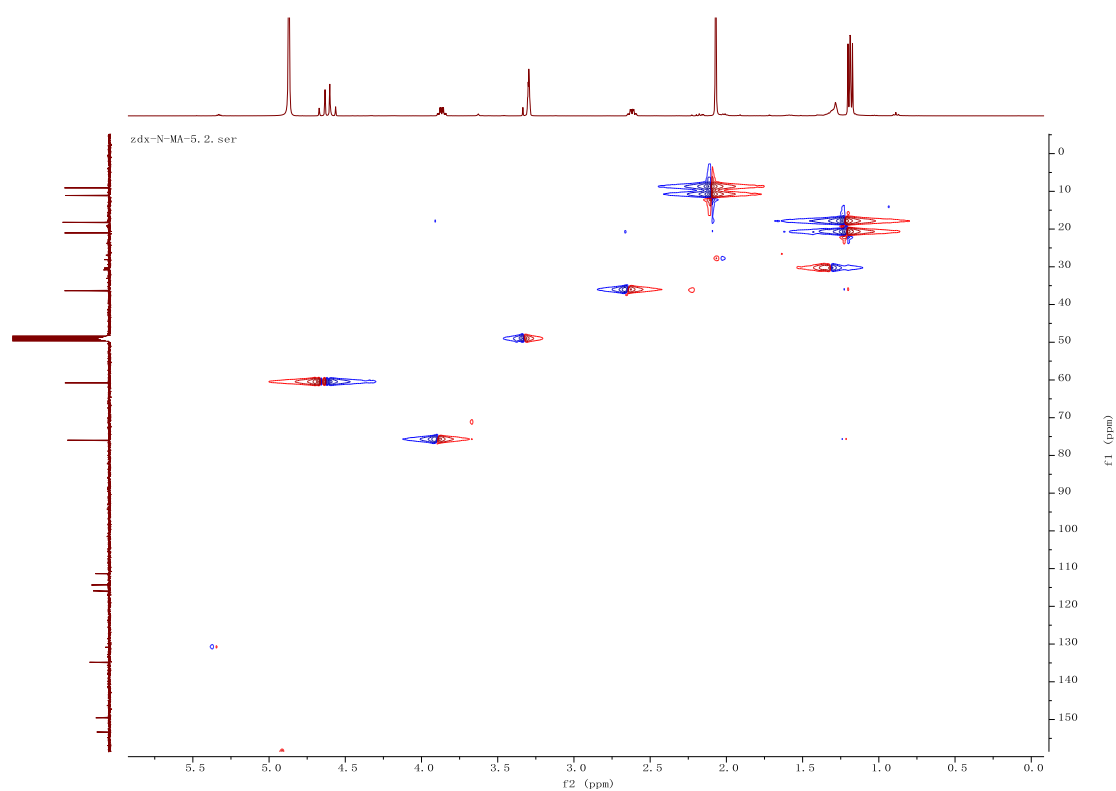


Figure S18. HMQC (methanol- d_4) spectrum of compound **3**

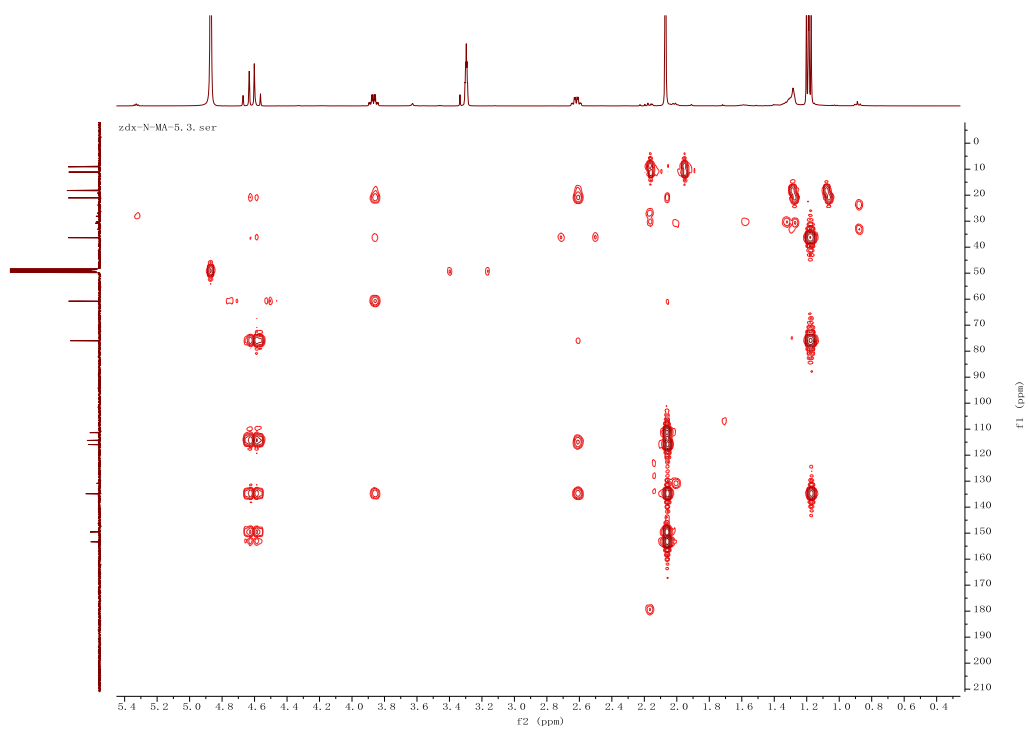


Figure S19. HMBC (methanol- d_4) spectrum of compound **3**

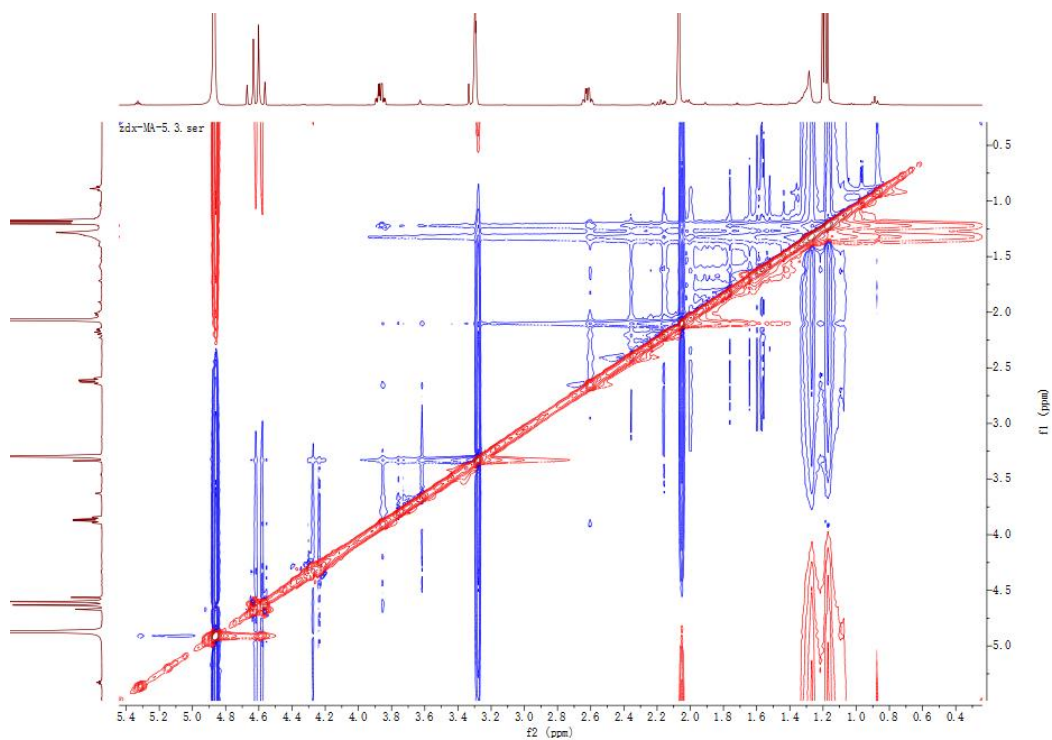


Figure S20. NOESY (methanol- d_4) spectrum of compound **3**

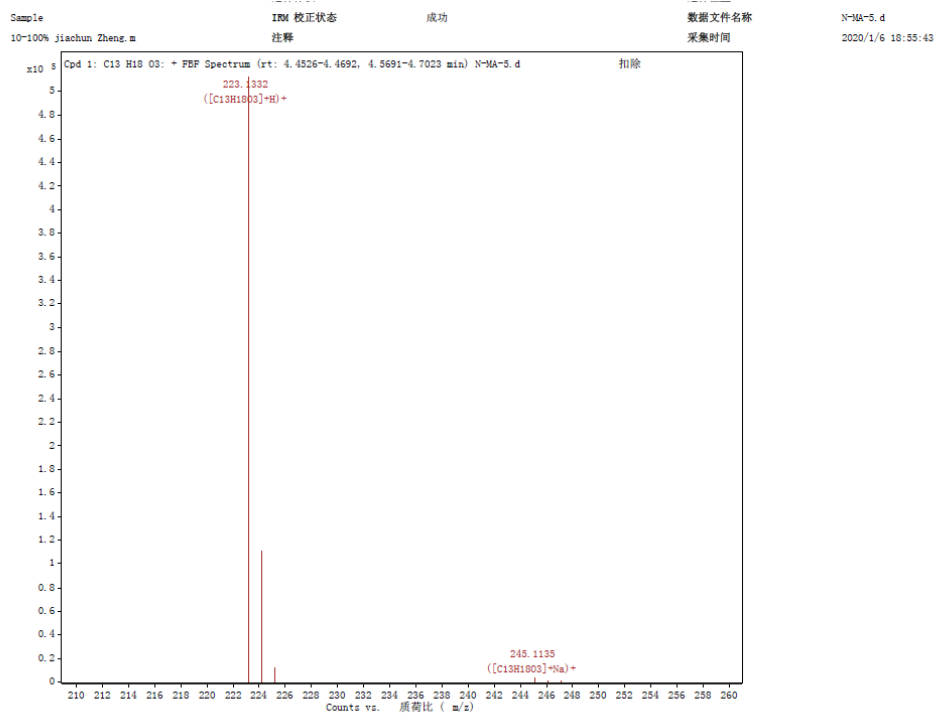


Figure S21. HR-ESI-MS spectrum of compound **3**

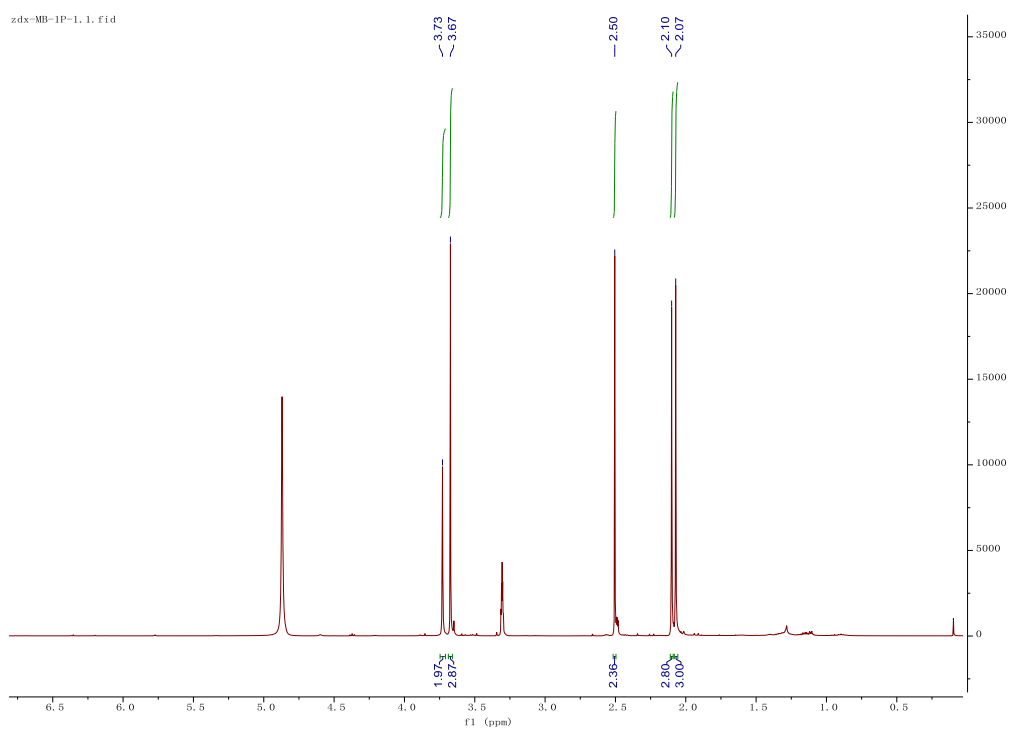


Figure S22. 1H NMR (400 MHz, methanol- d_4) spectrum of compound **4**

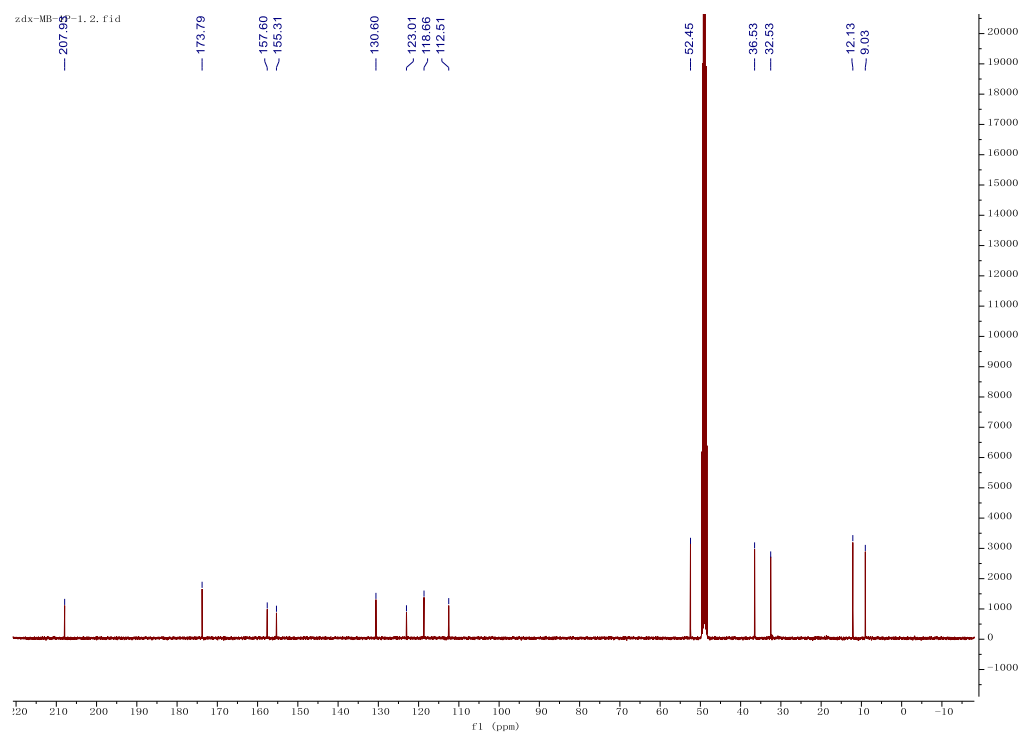


Figure S23. ^{13}C NMR (100 MHz, methanol- d_4) spectrum of compound **4**

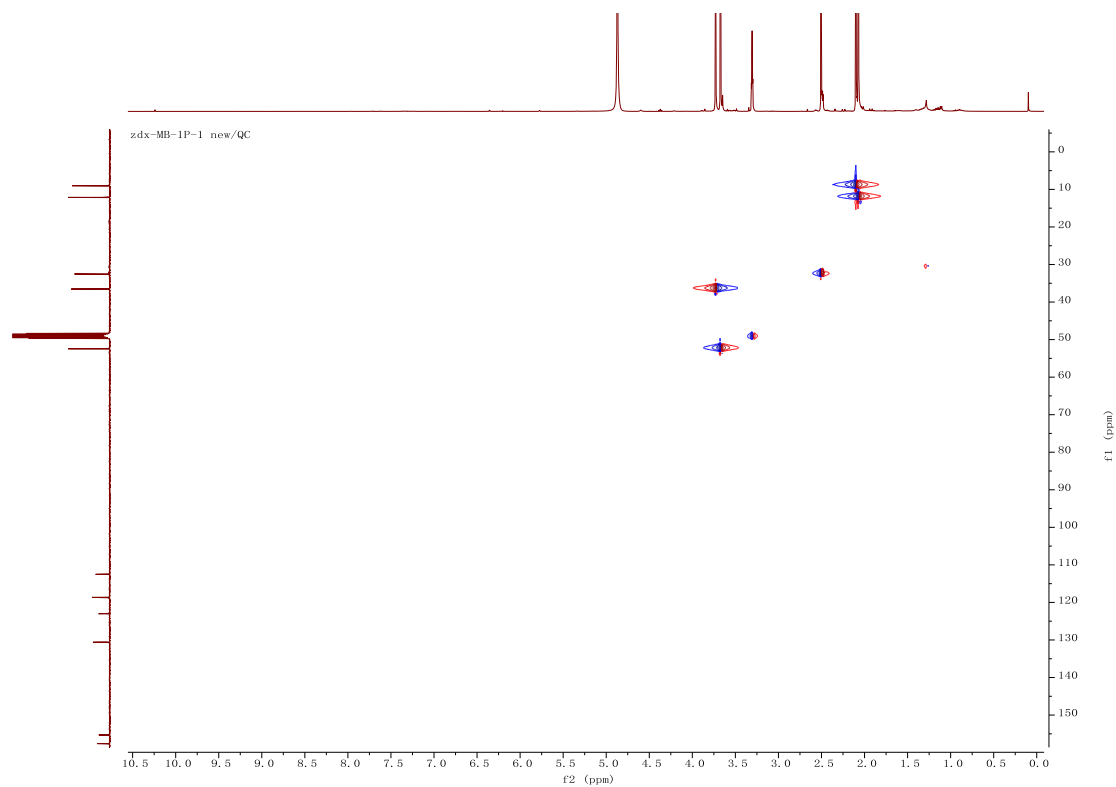


Figure S24. HMQC (methanol- d_4) spectrum of compound **4**

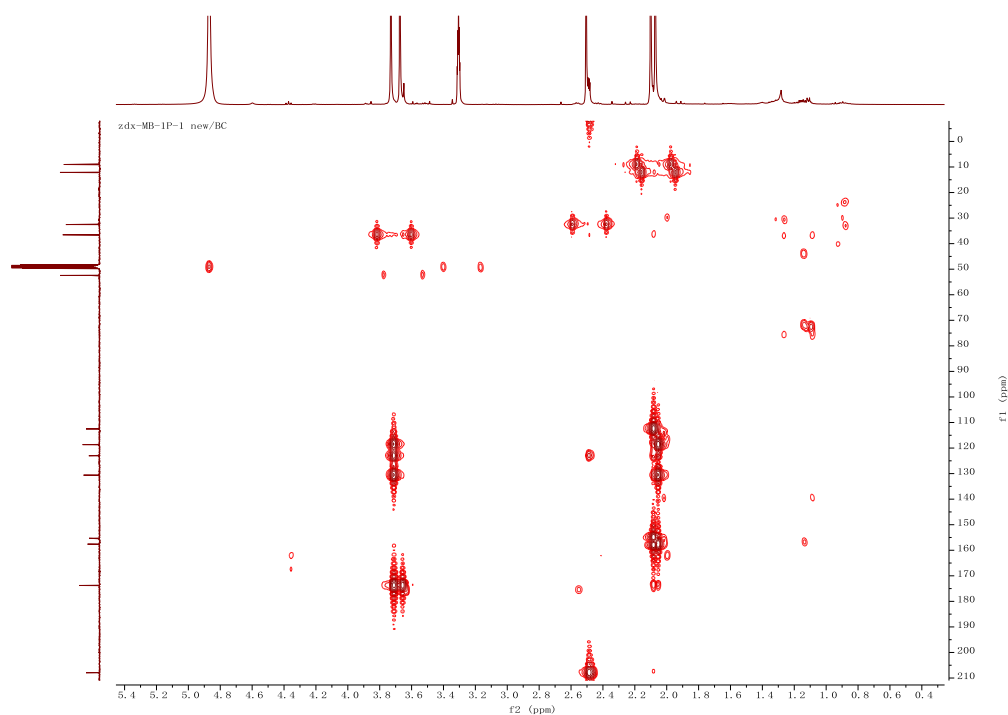


Figure S25. HMBC (methanol- d_4) spectrum of compound **4**

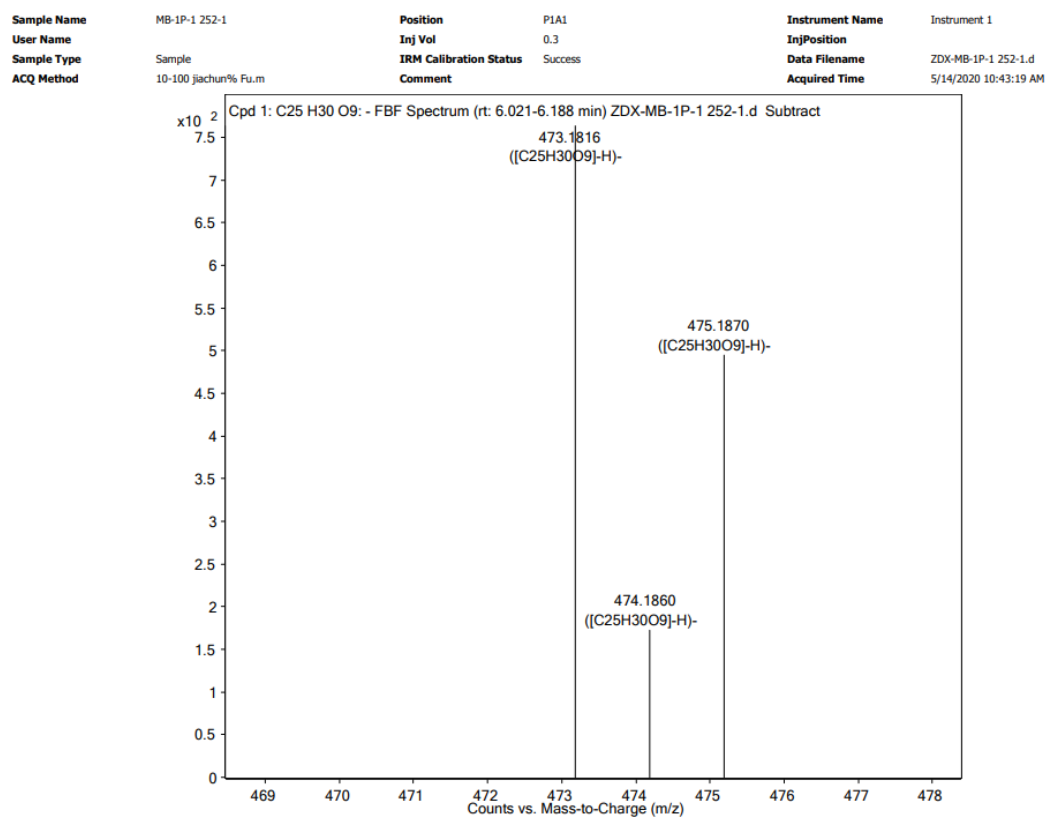


Figure S26. HR-ESI-MS spectrum of compound **4**

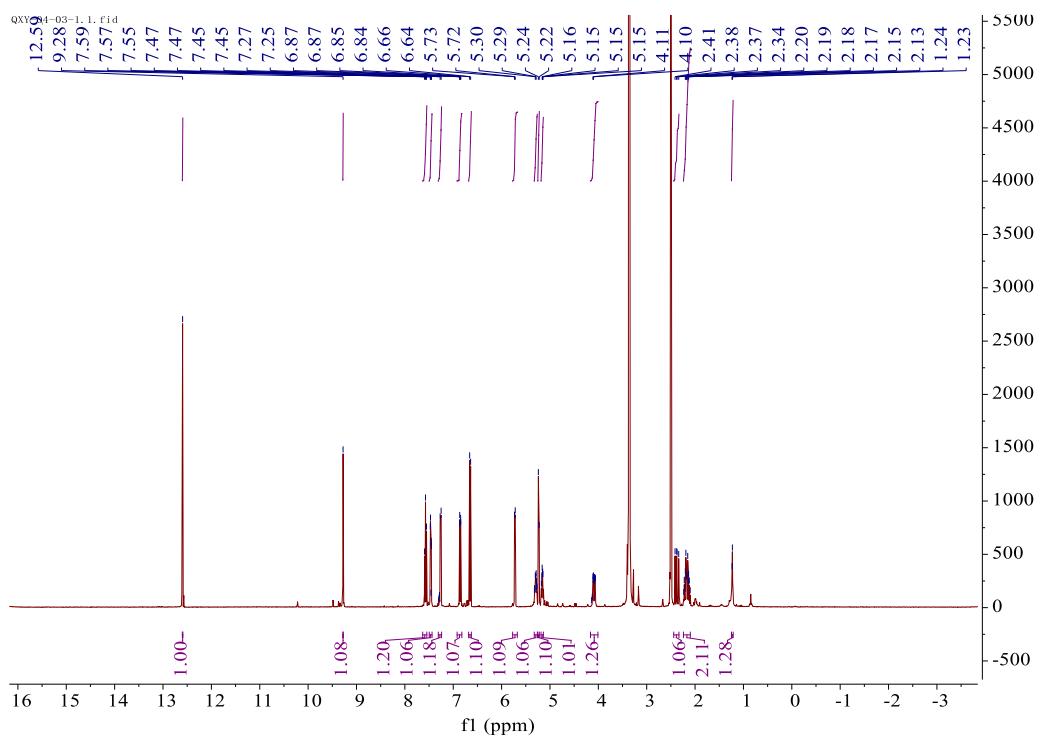


Figure S27. ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of compound **5**

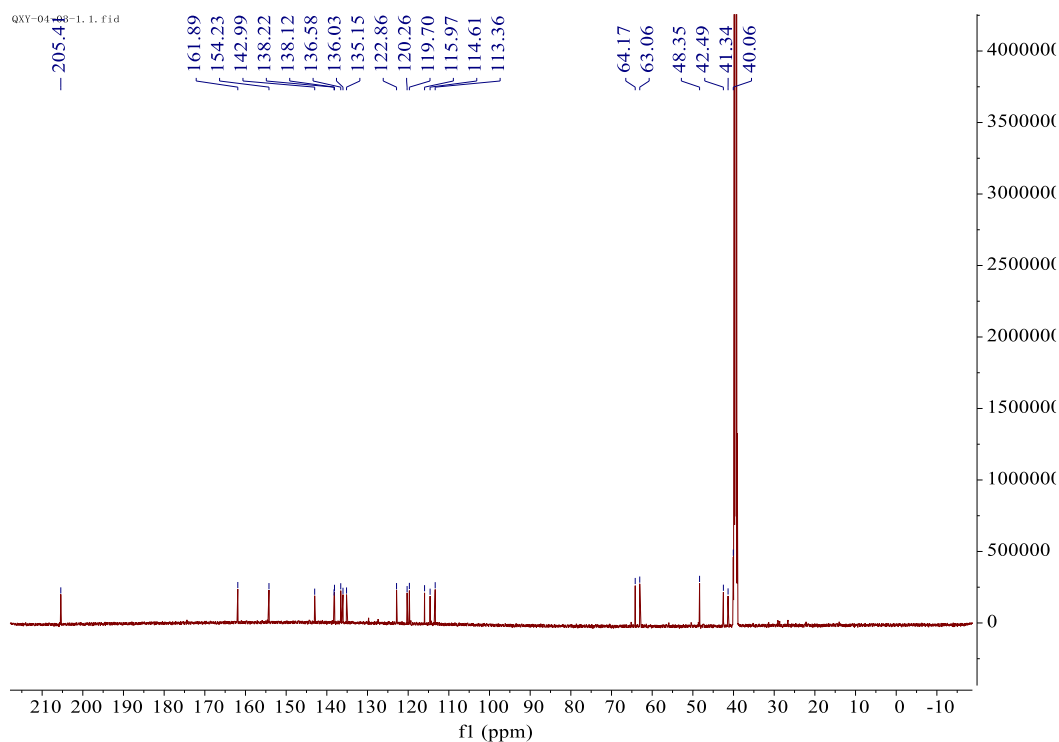


Figure S28. ¹³C NMR (150 MHz, DMSO-*d*₆) spectrum of compound **5**

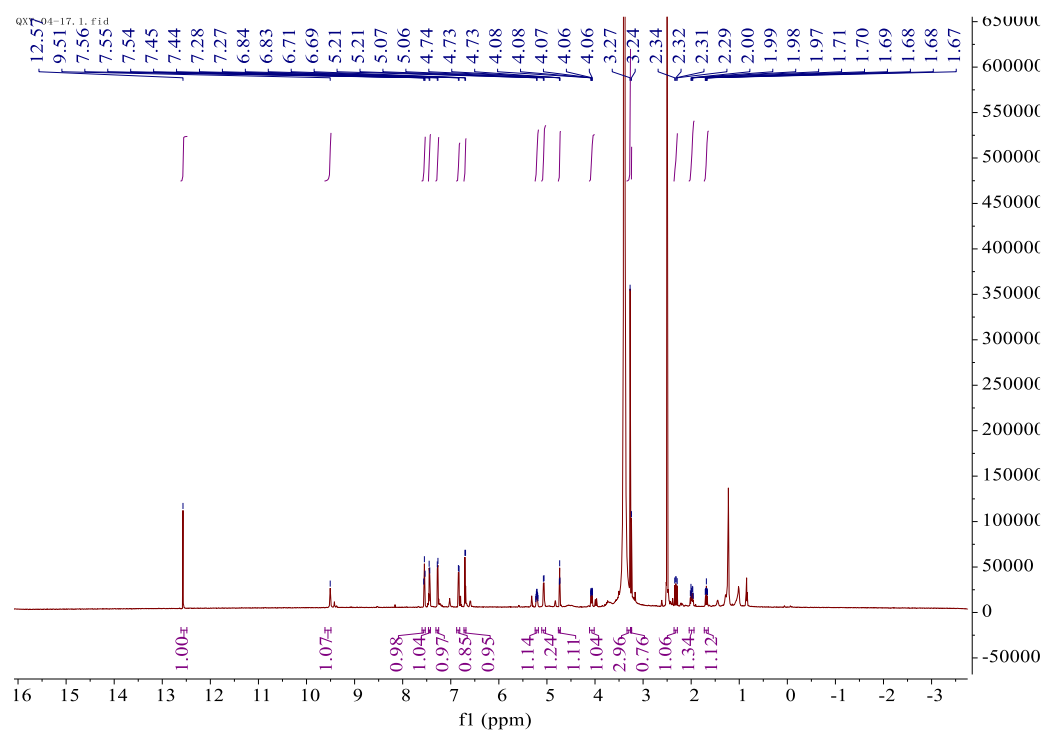


Figure S29. ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of compound **6**

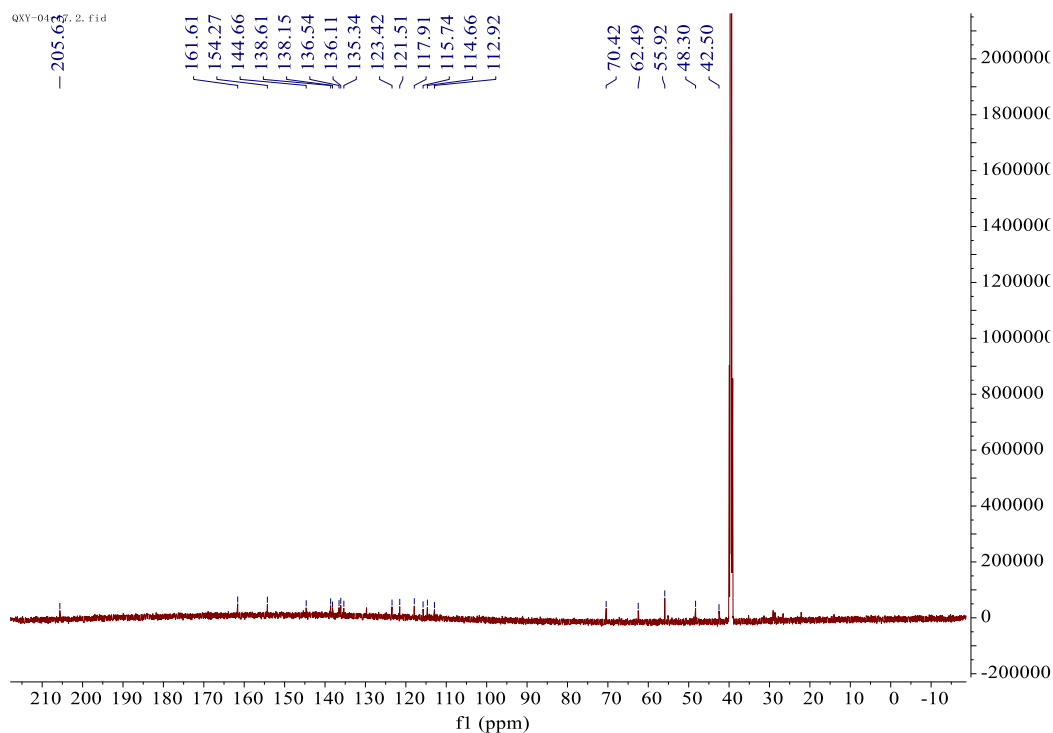


Figure S30. ¹³C NMR (150 MHz, DMSO-*d*₆) spectrum of compound **6**

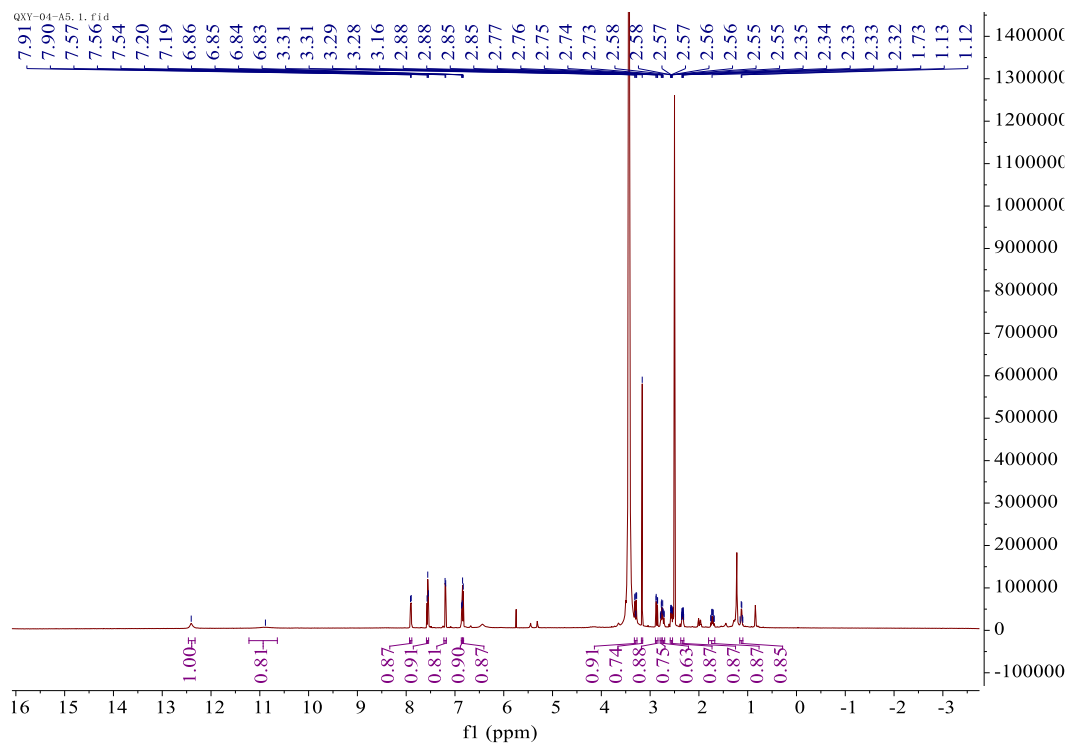


Figure S31. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of compound **7**

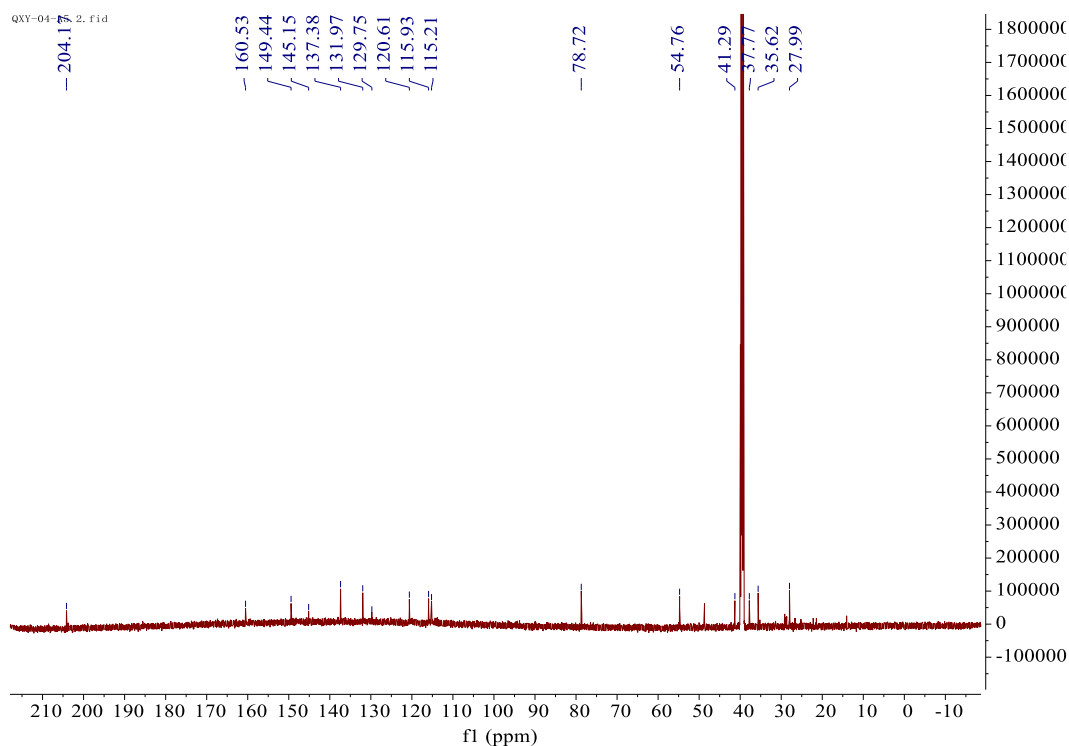


Figure S32. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of compound **7**

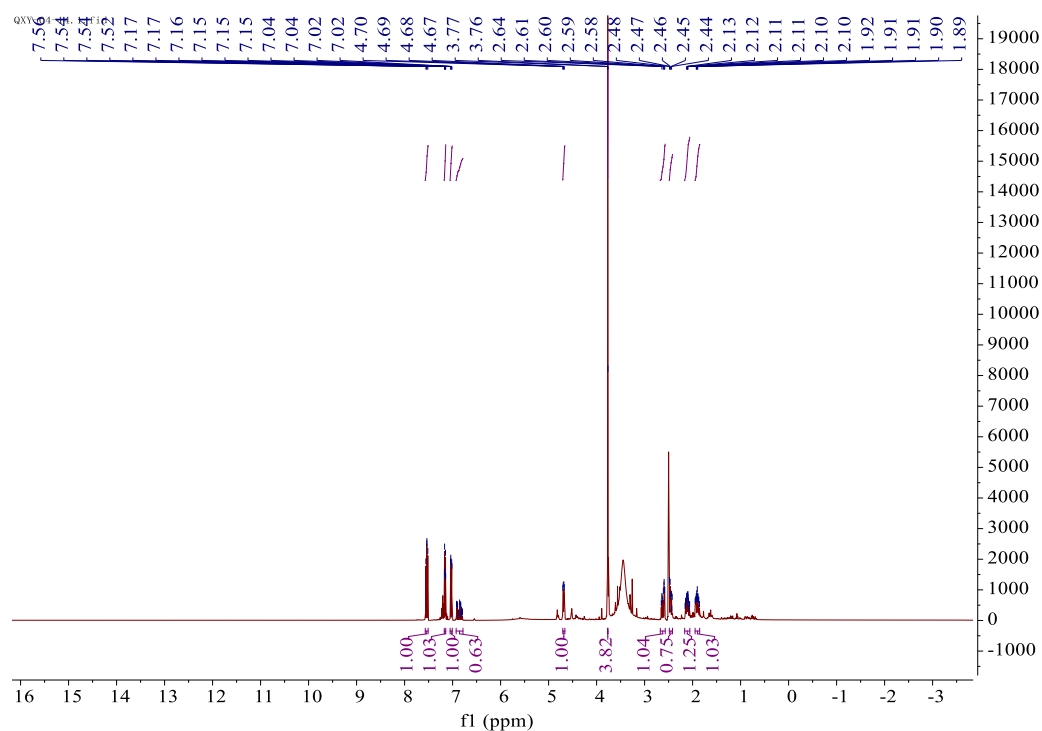


Figure S33. ¹H NMR (600 MHz, DMSO-*d*₆) spectrum of compound **8**

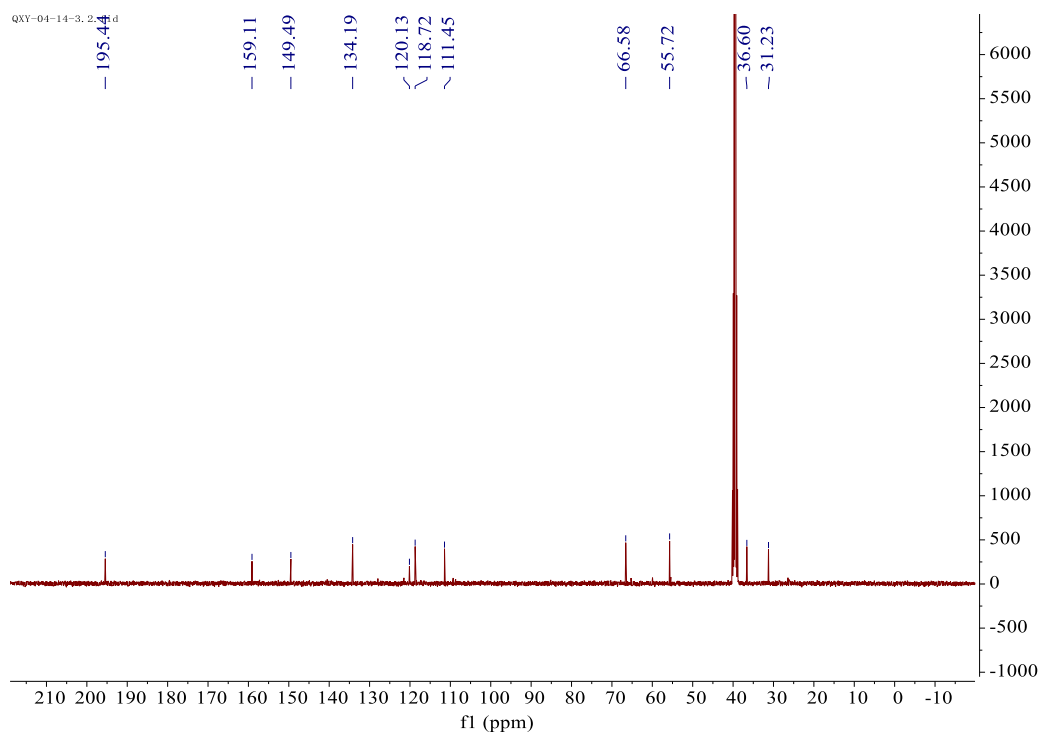


Figure S34. ¹³C NMR (150 MHz, DMSO-*d*₆) spectrum of compound **8**

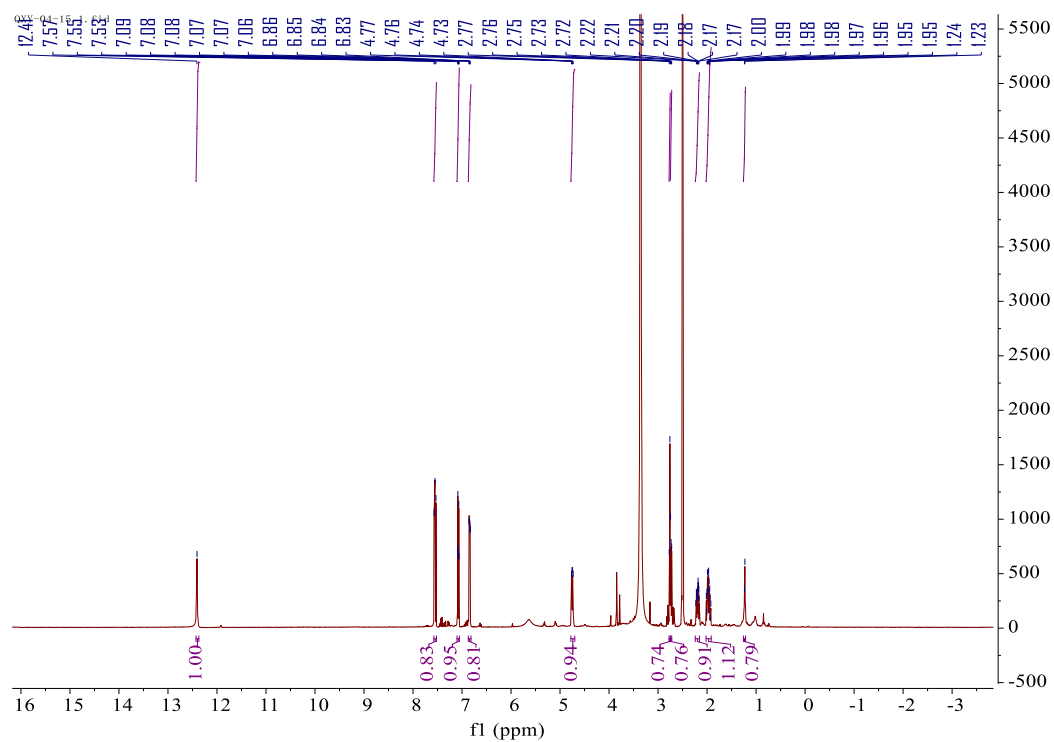


Figure S35. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of compound **9**

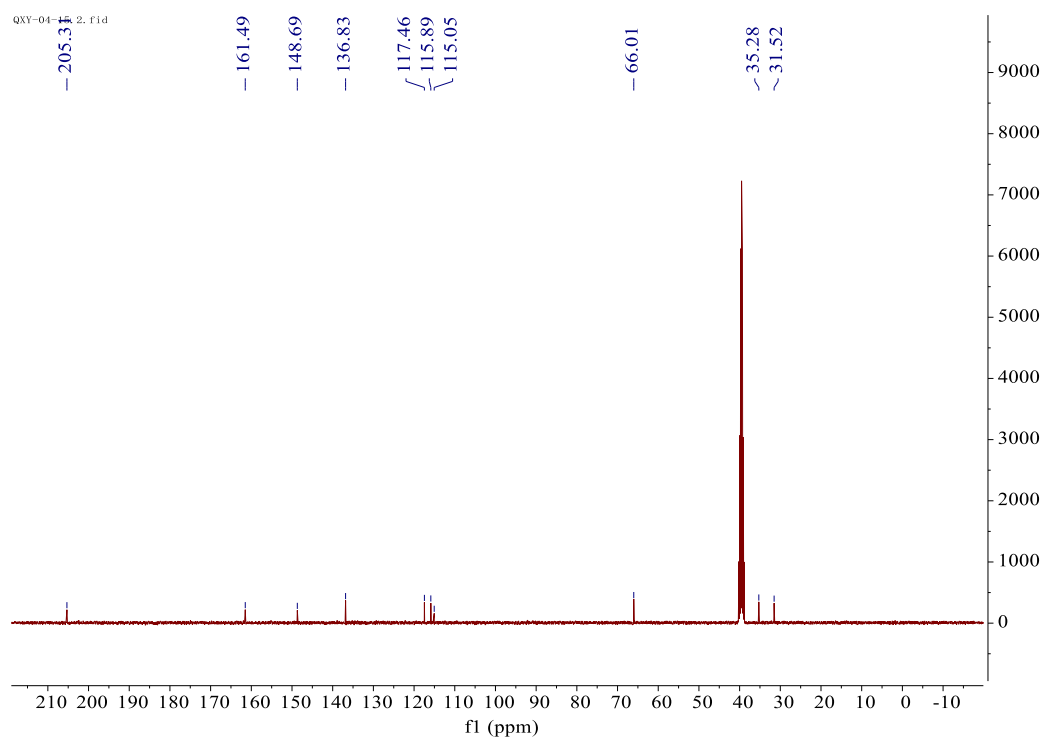


Figure S36. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of compound **9**

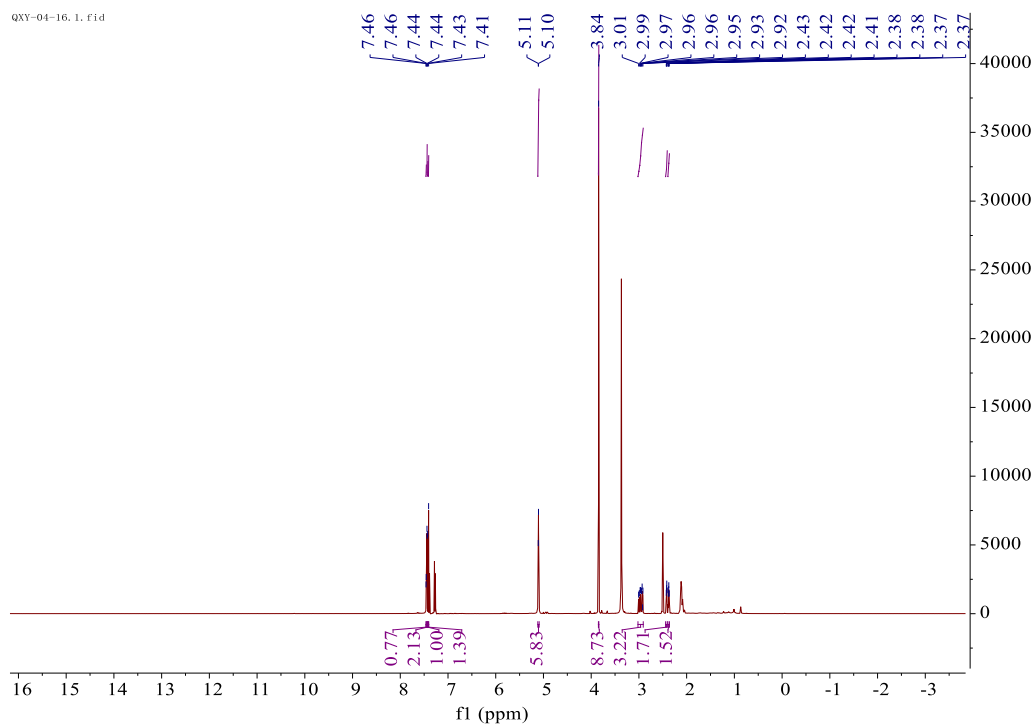


Figure S37. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of compound **10**

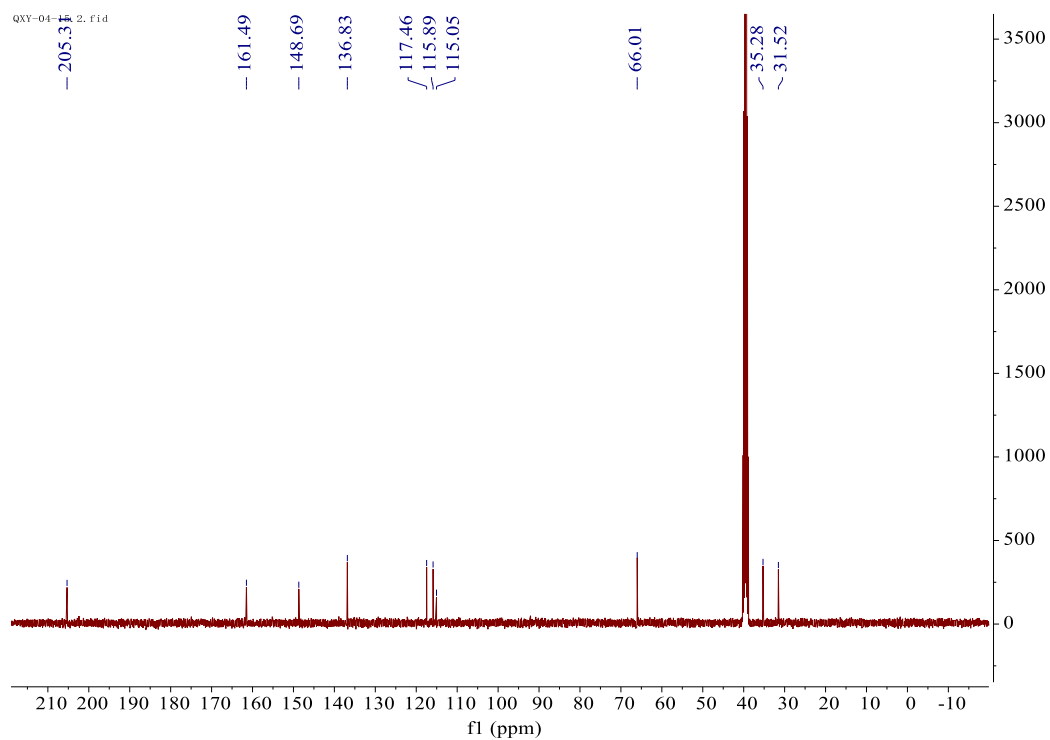


Figure S38. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of compound **10**

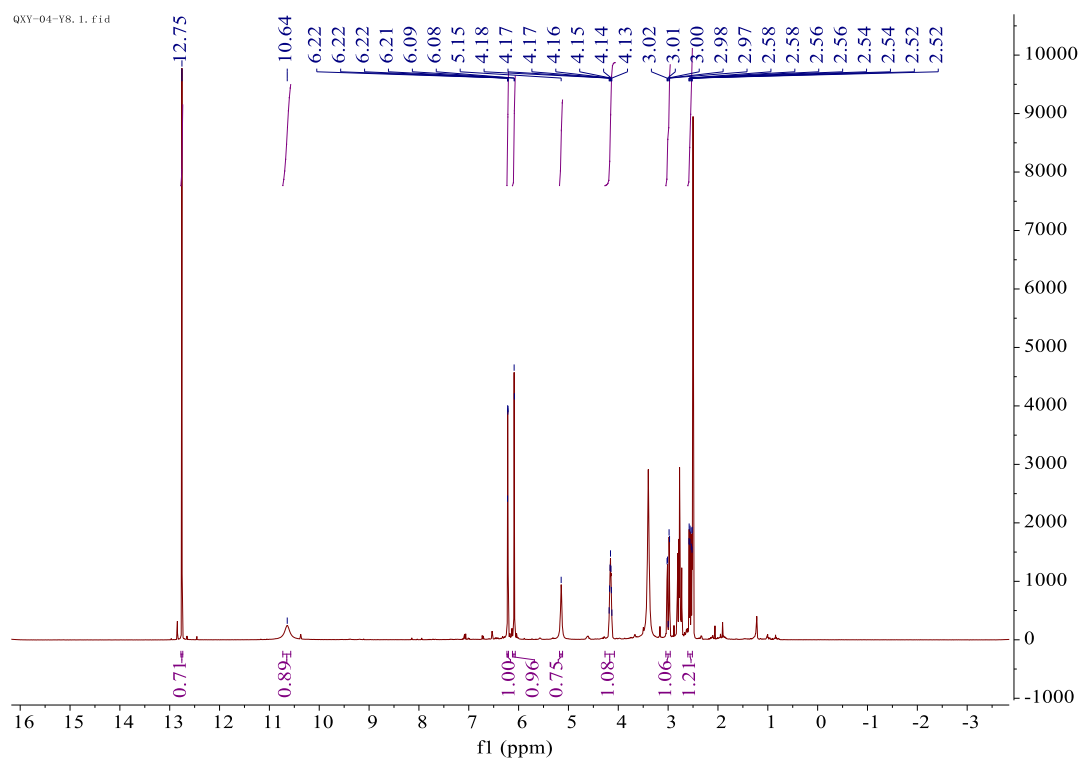


Figure S39. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of compound **11**

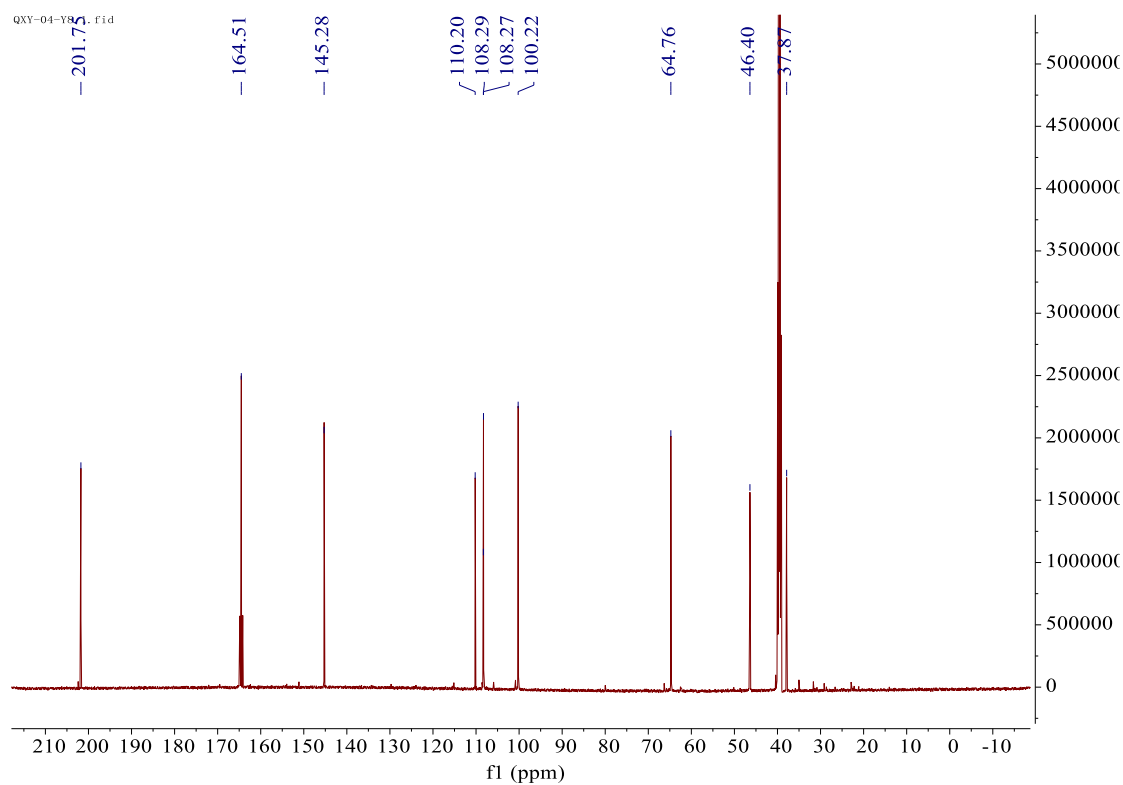


Figure S40. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of compound **11**

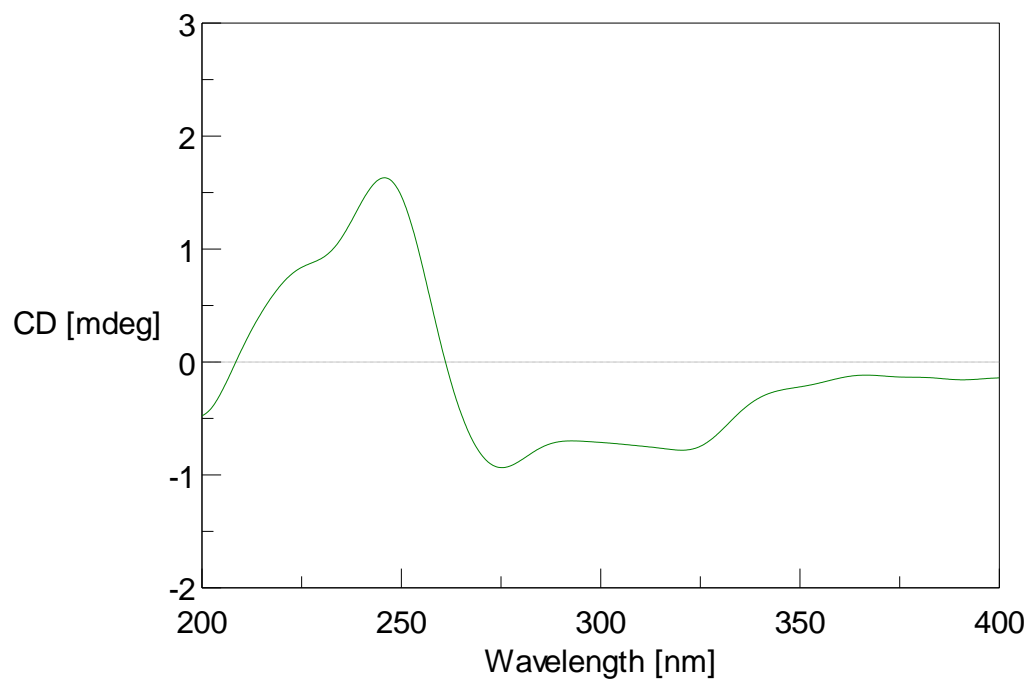
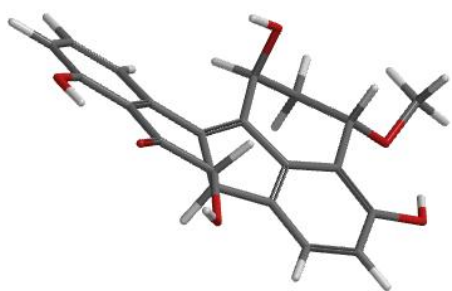
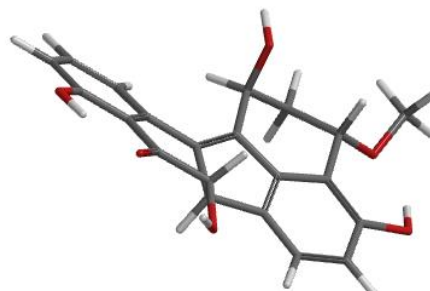


Figure S41. Experimental ECD of **1**

ECD calculation of **1**



Conformer **1-1** 0 kJ/mol, 94.9%



Conformer **1-2** 8.97 kJ/mol, 2.6%

ECD calculation of **1** model

Table S1. Energy minimized coordinates of **1-1** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z

C	0	0	0
C	0	0	1.390507
C	1.206981	0	2.106643
C	2.435433	0.011046	1.414218
C	2.416908	-0.01618	0.012603
C	1.208333	-0.01532	-0.68895
C	1.182857	-0.01663	3.596701
C	2.496006	0.01787	4.375469
C	3.621834	-0.62	3.570399
C	3.686163	0.007639	2.176478
C	5.71358	0.358932	3.096434
C	5.00129	-0.31977	4.083963
C	5.596883	-0.61444	5.296634
C	6.924193	-0.21415	5.490024
C	7.623367	0.468978	4.481464
C	7.025117	0.780571	3.258038
C	7.644135	1.605848	2.153716
C	7.032059	1.23582	0.786095
C	5.496551	1.331406	0.785751
C	4.885922	0.569094	1.915646
O	-1.2326	-0.00189	1.98855
O	0.097144	-0.03538	4.18465
O	5.131145	2.70405	0.905549
O	9.064774	1.379563	2.14801
C	9.789609	2.437488	1.527738
O	8.922779	0.802111	4.744486
O	2.29727	-0.69339	5.602909
H	3.499348	-1.70794	3.492701
H	-0.94203	-0.00297	-0.54342
H	3.335583	-0.07343	-0.56278
H	1.209366	-0.03808	-1.77727
H	2.71017	1.064994	4.626463
H	5.058044	-1.14347	6.077043
H	7.424895	-0.43591	6.429234
H	7.445128	2.660298	2.388724
H	7.435844	1.901739	0.014898
H	7.343498	0.21897	0.508904
H	5.137821	0.978573	-0.18247
H	-1.1055	-0.0272	2.963725
H	4.162019	2.735951	0.981187
H	9.593596	3.387558	2.033783
H	10.85641	2.213161	1.614878
H	9.541972	2.5143	0.465986
H	9.328408	1.017305	3.8788

H	1.422129	-0.41498	35 5.939153
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Table S2. Energy minimized coordinates of **1-2** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z
C	0	0	0
C	0	0	1.39036
C	1.208314	0	2.106162
C	2.434766	0.011195	1.4135
C	2.416841	-0.01482	0.012184
C	1.208516	-0.01438	-0.68966
C	1.185836	-0.02434	3.595559
C	2.500513	-0.00905	4.37358
C	3.619963	-0.64814	3.560288
C	3.6858	-0.00013	2.176754
C	5.709831	0.343152	3.10552
C	5.002476	-0.36237	4.077205
C	5.602122	-0.68786	5.279259
C	6.928059	-0.28925	5.480262
C	7.622909	0.424597	4.488822
C	7.018424	0.768136	3.277393
C	7.623915	1.635001	2.198468
C	7.014391	1.30417	0.818939
C	5.477582	1.376779	0.821701
C	4.879731	0.578043	1.93119
O	-1.23221	-0.00539	1.98848
O	0.099909	-0.03923	4.18555
O	5.074258	2.732929	0.992669
O	9.046687	1.426164	2.177066
C	9.759489	2.535733	1.637207
O	8.921259	0.75551	4.757317
O	2.295748	-0.73474	5.591916
H	3.490192	-1.73369	3.468109

H	-0.94136	-0.00223	-0.54395
H	3.337578	-0.06742	-0.5605
H	1.210372	-0.03475	-1.77704
H	2.723185	1.032424	4.636203
H	5.064715	-1.23631	6.047377
H	7.431323	-0.53486	6.41203
H	7.411593	2.678913	2.468305
H	7.409804	2.002028	0.071882
H	7.339465	0.302635	0.50753
H	5.112459	1.036988	-0.15029
H	-1.10189	-0.02087	2.963507
H	5.180696	3.177426	0.134761
H	9.572082	3.435864	2.229555
H	10.82813	2.307923	1.684495
H	9.489875	2.705184	0.591324
H	9.324048	0.994864	3.896949
H	1.425197	-0.44659	5.933152

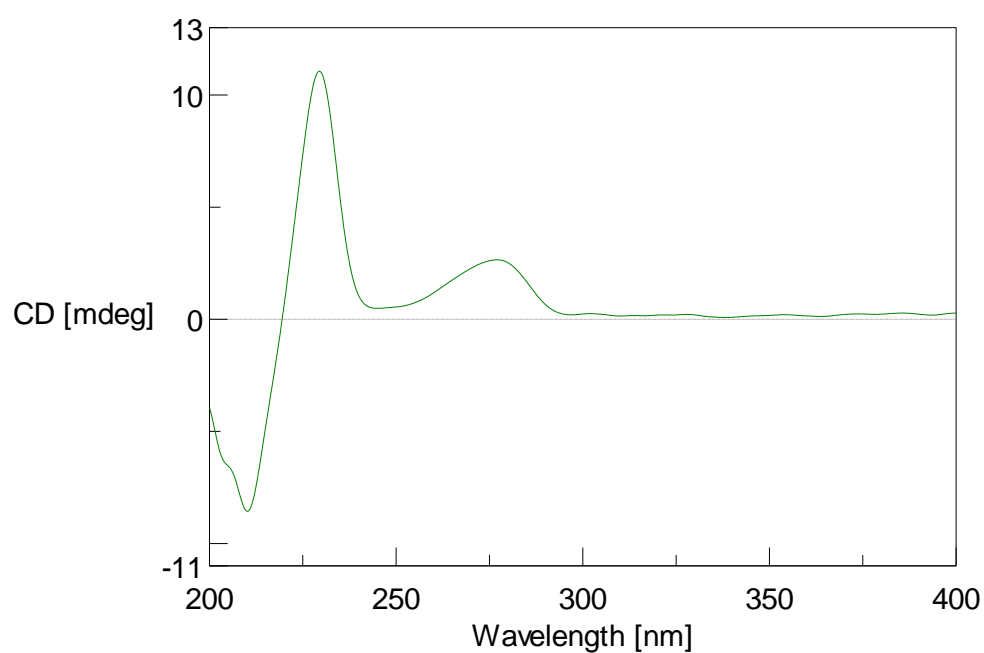
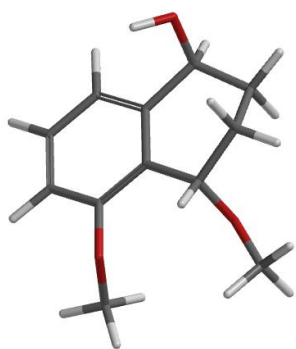
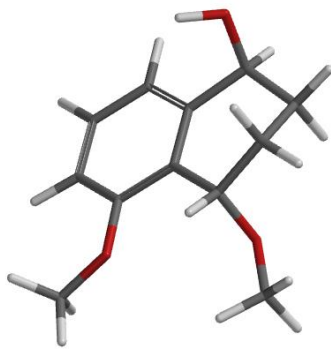


Figure S42. Experimental ECD of **2**

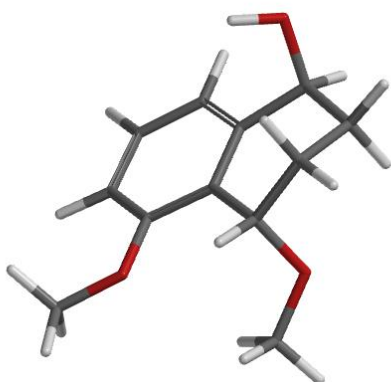
ECD calculation of **2**



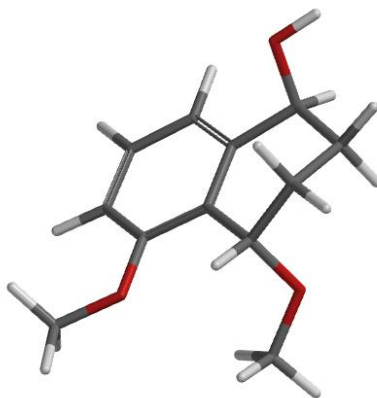
Conformer **2-1**, 0 kJ/mol, 32.9%



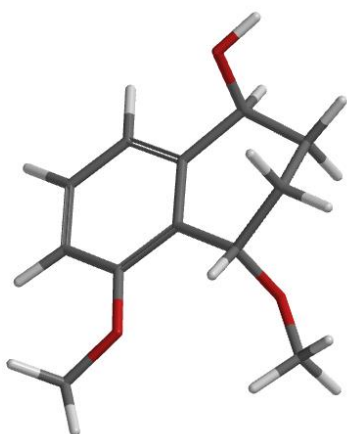
Conformer **2-2**, 0.22kJ/mol, 30.1%



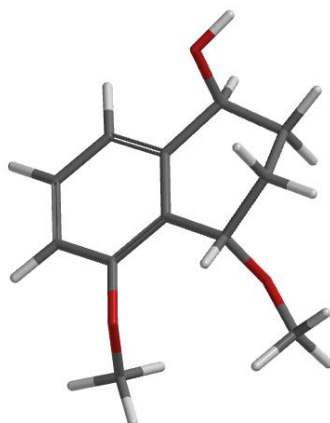
Conformer **2-3**, 0.88 kJ/mol, 23.1%



Conformer **2-4**, 4.94 kJ/mol, 4.6%



Conformer **2-5**, 5.32 kJ/mol, 3.8%



Conformer **2-5**, 7.64 kJ/mol, 3.4%

ECD calculation of **2** model

Table S3. Energy minimized coordinates of **2-1** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z

C	0	0	0
C	0	0	1.391134
C	1.21166	0	2.087532
C	2.441338	0.046246	1.40872
C	2.435458	0.041116	-0.00293
C	1.209451	0.017754	-0.6923
C	3.740393	0.049162	2.189915
C	4.931253	0.534886	1.354319
C	4.971907	-0.18899	0.009458
C	3.716925	0.124774	-0.8034
O	1.205523	0.025857	3.460316
C	0.73717	-1.21778	3.985219
O	3.853153	1.444629	-1.33844
O	3.981354	-1.30406	2.605414
C	4.600943	-1.37859	3.882407
H	-0.93977	-0.00491	-0.54444
H	-0.94314	0.008137	1.928573
H	1.197254	0.025369	-1.78166
H	3.63623	0.710816	3.059581
H	4.855274	1.617175	1.189872
H	5.871771	0.350395	1.883665
H	5.866586	0.125485	-0.541
H	5.050527	-1.26998	0.175066
H	3.668014	-0.56714	-1.65117
H	0.990386	-1.24611	5.049086
H	-0.3516	-1.29167	3.896328
H	1.220292	-2.07334	3.500251
H	3.122825	1.98599	-0.99305
H	3.945064	-0.95819	4.650864
H	4.775582	-2.43211	4.116794
H	5.56309	-0.85895	3.88148

Table S4. Energy minimized coordinates of **2-2** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z
C	0	0	0
C	0	0	1.393617
C	1.206343	0	2.102885
C	2.433797	0.015947	1.404252
C	2.427887	0.014935	-0.00959
C	1.203981	0.009319	-0.69718
C	3.743061	-0.02406	2.171678
C	4.93728	0.457668	1.339905

C	4.963927	-0.24974	-0.01287
C	3.708269	0.084126	-0.81461
O	1.290466	0.017797	3.47212
C	0.111507	-0.31227	4.196967
O	3.859132	1.405759	-1.34368
O	3.971382	-1.39013	2.545205
C	4.484326	-1.51499	3.86347
H	-0.94156	-0.00275	-0.54378
H	-0.95895	0.006519	1.8992
H	1.189187	0.017305	-1.78576
H	3.666611	0.621063	3.057717
H	4.877677	1.543164	1.190791
H	5.874386	0.249808	1.867386
H	5.859297	0.062391	-0.56471
H	5.03328	-1.33361	0.138756
H	3.645489	-0.60125	-1.66754
H	-0.3026	-1.2733	3.872982
H	0.385233	-0.4071	5.252603
H	-0.63156	0.487626	4.117662
H	3.145506	1.95727	-0.98119
H	3.757524	-1.14615	4.593703
H	4.668386	-2.57403	4.061817
H	5.429272	-0.9716	3.965129

Table S5. Energy minimized coordinates of **2-3** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z
C	0	0	0
C	0	0	1.393825
C	1.205227	0	2.103934
C	2.435028	-0.01129	1.406554
C	2.428853	0.025852	-0.0077
C	1.203188	0.022079	-0.69509
C	3.753763	-0.08567	2.161615
C	4.87597	0.595292	1.365576
C	4.991086	-0.02868	-0.02629
C	3.700637	0.167435	-0.81782
O	1.289375	0.026498	3.472921
C	0.07338	0.017771	4.210209
O	3.739574	1.483291	-1.3847
O	4.167569	-1.45012	2.340137
C	3.545346	-2.10565	3.434378
H	-0.9415	-0.0002	-0.5441

H	-0.96111	0.000969	1.895862
H	1.190411	0.054802	-1.78358
H	3.694068	0.423175	3.132226
H	4.68994	1.672721	1.281975
H	5.831399	0.462942	1.887786
H	5.837797	0.423986	-0.55644
H	5.206514	-1.10034	0.06773
H	3.689386	-0.54261	-1.65272
H	-0.49986	-0.89364	4.015203
H	0.328674	0.027799	5.274392
H	-0.51939	0.914925	4.002788
H	3.102607	2.034495	-0.89972
H	2.500269	-2.33162	3.208065
H	4.061991	-3.05543	3.596532
H	3.624412	-1.51167	4.349925

Table S6. Energy minimized coordinates of **2-4** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z
C	0	0	0
C	0	0	1.39313
C	1.205978	0	2.102889
C	2.435499	-0.02052	1.404328
C	2.430791	0.007941	-0.01006
C	1.204708	0.013161	-0.69483
C	3.753876	-0.0772	2.160646
C	4.870041	0.601671	1.354305
C	4.996635	-0.05009	-0.02141
C	3.704566	0.108272	-0.82166
O	1.290087	0.028658	3.472386
C	0.075286	0.113203	4.205429
O	3.705699	1.399636	-1.43843
O	4.181259	-1.43596	2.35882
C	3.546774	-2.08752	3.448358
H	-0.94036	0.009923	-0.54472
H	-0.96157	0.0068	1.894288
H	1.191835	0.053778	-1.78316
H	3.690834	0.4439	3.12405
H	4.671519	1.675437	1.248033
H	5.824933	0.491655	1.88185
H	5.841862	0.396852	-0.55824
H	5.224115	-1.11679	0.096755
H	3.684738	-0.63959	-1.62303

H	-0.54339	-0.77553	4.046995
H	0.330433	0.154009	5.268868
H	-0.47223	1.029071	3.960701
H	4.481479	1.435438	-2.02064
H	4.070798	-3.03063	3.628502
H	3.604771	-1.48494	4.358468
H	2.50763	-2.32697	3.206124

Table S7. Energy minimized coordinates of **2-5** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z
C	0	0	0
C	0	0	1.39441
C	1.20638	0	2.102692
C	2.433637	0.006675	1.402545
C	2.429633	-0.00343	-0.01184
C	1.204067	0.001517	-0.69619
C	3.743189	-0.01291	2.169901
C	4.930803	0.467335	1.328425
C	4.968252	-0.27278	-0.00654
C	3.707534	0.024735	-0.81792
O	1.294148	0.018389	3.472861
C	0.094291	-0.19113	4.20518
O	3.818314	1.327104	-1.39306
O	3.991046	-1.37179	2.559692
C	4.459661	-1.47381	3.896653
H	-0.94087	0.009713	-0.54351
H	-0.95943	0.011256	1.898569
H	1.190864	0.021495	-1.78428
H	3.663477	0.643951	3.045597
H	4.857595	1.548233	1.152733
H	5.870016	0.283027	1.861599
H	5.861753	0.033493	-0.56362
H	5.048835	-1.35132	0.171988
H	3.63641	-0.69791	-1.64078
H	-0.59311	0.652971	4.082023
H	-0.3835	-1.13703	3.928706
H	0.357367	-0.25093	5.26623
H	4.59521	1.316464	-1.9746
H	3.698584	-1.1172	4.597422
H	4.660616	-2.52611	4.111282
H	5.387085	-0.90756	4.026049

Table S8. Energy minimized coordinates of **2-6** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z
C	0	0	0
C	0	0	1.390728
C	1.21056	0	2.08642
C	2.440954	0.041706	1.40626
C	2.436806	0.025412	-0.00599
C	1.209045	0.009848	-0.69226
C	3.738965	0.069619	2.186019
C	4.924248	0.550821	1.34054
C	4.975017	-0.20878	0.016524
C	3.716679	0.066797	-0.80737
O	1.206518	0.0297	3.459299
C	0.72762	-1.20728	3.987844
O	3.81354	1.367172	-1.38997
O	3.998725	-1.27283	2.626752
C	4.588722	-1.31451	3.91871
H	-0.9395	0.006017	-0.54583
H	-0.94346	0.016445	1.928087
H	1.198654	0.02862	-1.78131
H	3.629801	0.747753	3.042915
H	4.835279	1.627561	1.14717
H	5.86594	0.390766	1.876745
H	5.869212	0.097004	-0.53953
H	5.063956	-1.28405	0.21185
H	3.660215	-0.66136	-1.62444
H	0.980196	-1.23496	5.051984
H	-0.36107	-1.27417	3.899681
H	1.204925	-2.0685	3.505106
H	4.592712	1.364205	-1.96859
H	3.905917	-0.89796	4.665063
H	4.783016	-2.35926	4.17238
H	5.538422	-0.77057	3.931473

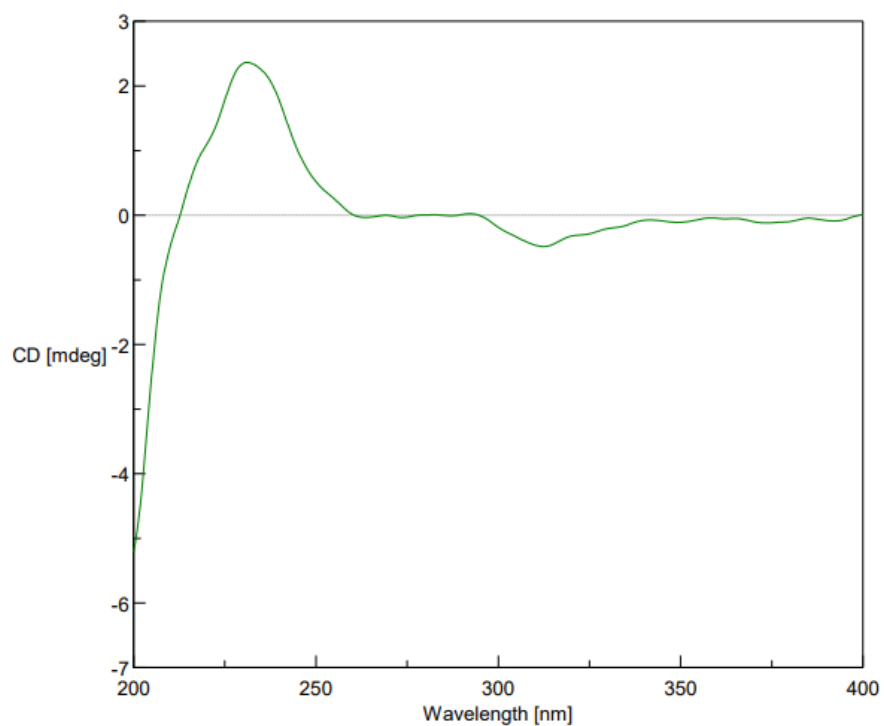
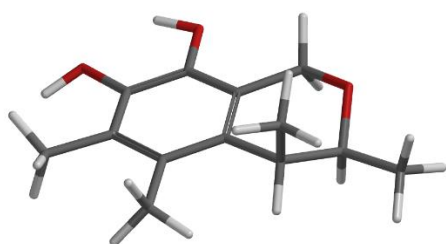
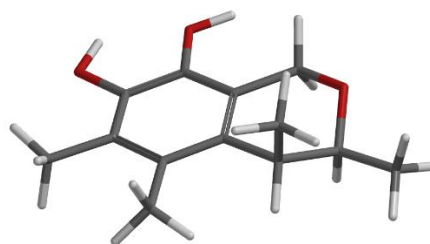


Figure S43. Experimental ECD of **3**

ECD calculation of **3**



Conformer **3-1** 0 kJ/mol, 96.9%



Conformer **3-2** 8.94 kJ/mol, 2.6%

ECD calculation of **3** model

Table S9. Energy minimized coordinates of **3-1** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z

C	0	0	0
C	0	0	1.424333
C	1.238133	0	2.134091
C	2.461205	-0.02906	1.424601
C	2.429986	-0.09551	0.035242
C	1.226265	-0.09308	-0.66766
O	1.342512	-0.19382	-2.03268
O	3.601455	-0.17519	-0.6721
C	-1.28973	0.067066	-0.77867
C	3.797712	-0.05007	2.129669
C	-1.32384	0.053396	2.154767
C	1.315216	0.074584	3.659723
C	2.661602	-0.51232	4.144461
C	1.1032	1.5289	4.104947
O	3.731777	0.211621	3.536074
C	2.849434	-0.43819	5.655081
H	0.481479	-0.4538	-2.39748
H	3.317656	-0.18026	-1.60806
H	-2.06059	0.634351	-0.24891
H	-1.15432	0.591063	-1.73098
H	-1.66026	-0.94336	-0.97621
H	4.458088	0.713013	1.702868
H	4.269869	-1.02996	1.990654
H	-1.72137	1.072926	2.127533
H	-2.04508	-0.63076	1.694994
H	-1.25844	-0.2581	3.197574
H	0.536002	-0.55539	4.099502
H	2.734939	-1.57006	3.853551
H	1.058296	1.605264	5.19569
H	0.161947	1.934453	3.71994
H	1.907282	2.182873	3.751101
H	2.964376	0.593784	6.001248
H	3.771491	-0.95708	5.941299
H	2.013617	-0.90598	6.184707

Table S10. Energy minimized coordinates of **3-2** model at the basis set def-SV(P) for all atoms(Å).

Atom	X	Y	Z

C	0	0	0
C	0	0	1.418143
C	1.240864	0	2.123133
C	2.471651	-0.0303	1.412336
C	2.437068	-0.0793	0.016179
C	1.222024	-0.06406	-0.66966
O	1.254905	-0.11574	-2.04008
O	3.556046	-0.14609	-0.7783
C	-1.28397	0.027769	-0.78949
C	3.790475	-0.06689	2.152467
C	-1.32642	0.063896	2.141828
C	1.303903	0.071377	3.650708
C	2.631831	-0.53903	4.147956
C	1.109318	1.527312	4.096121
O	3.71702	0.174529	3.555867
C	2.803085	-0.47834	5.661376
H	2.207662	-0.15388	-2.25801
H	4.356909	-0.10674	-0.23402
H	-1.97782	0.769377	-0.38013
H	-1.1242	0.309902	-1.83538
H	-1.75435	-0.96078	-0.77249
H	4.459762	0.700927	1.748175
H	4.262375	-1.04508	2.001595
H	-1.68929	1.096941	2.157927
H	-2.07249	-0.56876	1.650462
H	-1.27773	-0.29975	3.16854
H	0.509719	-0.54683	4.083642
H	2.694533	-1.59581	3.850045
H	1.057029	1.603848	5.186036
H	0.177637	1.947186	3.703818
H	1.926303	2.17021	3.748904
H	2.927509	0.549072	6.016053
H	3.714889	-1.01104	5.954041
H	1.954816	-0.93758	6.17757